Advanced Modeling and Computer Technologies for Fluvial Water Quality Research and Control

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INTRODUCTION

For solving the problems of study, analysis and quality management of the environment there is necessary operatively to treat great amount of measuring information on physical, chemical and biological parameters characteristic for them. To do it in a proper way, in conformity to the modern requirements, is possible only by wide use of modern mathematical methods and computers. For this purpose it is necessary to develop automated systems and universal program packages with developed mathematical methods consisting of self-learning algorithms requiring whenever it is possible minimum a prior information and having capability of adaptation to the most unexpected changes of the character of the investigated objects [1].

Among the most topical problems of monitoring of a natural water environment it is necessary to single out the following issues: simulation of pollutants transferring in water objects; methods of making decisions about condition of controlled objects and processes taking place in them; identification of sources of emergency pollution to take measures for their elimination. These problems are especially urgent in urban conditions because there exist great number of sources of pollution. Their solution is of great ecological and economical significance which makes possible to investigate the effect of different sources of pollution on ecological object separately from each other, as well as jointly, to predict outcomes of such an impact and consequences of the nature protection measures against the sources of pollution. With their help, the minimization of technical means, in particular, those of measurements, indispensable for the control and management of each source of pollution is reached. They are also actual for large plants and factories having biochemical clearing of sewages, on their design and ecological safe operation, as well as for detection of sites and shops producing the excess of sewages pollution.

Theoretical analysis of water pollution consequences, economic assessment of losses and creation of methodical principles on the basis of these investigations for the definition of efficiency of capital investments in nature protection measures are impossible without knowledge of the processes of pollutants diffusion. Development of scientifically reasonable programs of long-term planning of measures, directed to the reduction of discharges of different sources, evaluation of ecological perfection of various technologies, development of methods and tools for monitoring, prediction and management of environmental quality are inextricably connected with mathematical modeling of processes of transfer and diffusion of harmful impurities. On the other hand, availability of modern automated environmental management and monitoring systems open wide possibilities for using mathematical methods during study

and rational utilization of natural resources. Success of application of mathematical methods in the solution of separate problems, in many respects depends on adequacy of models used for description of real processes, taking place in the studied environment. Mathematical models describing formation and development in time of a state of environmental objects, are used as at pre-design stage of design development for monitoring systems (selection of a system structure, site-installation of stations – auto-analyzers, time-space decidability of measurement tools, etc.), so during their exploitation (algorithms for the evaluation of a state, forecasting, identification of emergency discharge sources, etc [1]).

A number of scientific works is dedicated to the development and application of mathematical models of water environment pollution (see chapters 1, 3). In general case depending on the studied problems through mathematical models, their structures, detailed study of the phenomenon, the volume of the used experimental information, mathematical models of the environmental pollution can be united in three large classes [1]: numerical (diffusive), statistical and imitative. Each of them has the advantages and disadvantages and in many respects depends on the rate of adequacy of conditions of studied process of pollution.

Numerical models based on the solution of relevant differential equations of diffusion and transfer of pollutants are most widely spread (see chapter 1). However, due to the fact that environmental objects are rather complex systems with a huge number of interrelated parameters, the operating evaluation of which as a rule, is not easy, the accuracy of the deterministic models is limited. They are constructed on the basis of analysis of physical-chemical and biological processes in the environment and reflect the development of these processes in time. Their advantage is the clearness of cause-effect relationship in these processes. The application is efficient at solving of particular, local in a space and time scale problems. The problem of application limits for these models has not been studied in detail till now, although in the work [2] is shown that of weather forecast-time interval by differential equations in principle cannot exceed 15 days. At appropriate selection of a structure and methods of identification, statistical models allow to predict with satisfactory accuracy during practically interesting time period at correct use of experimental data.

Statistical models, or so-called models “of a black box”, differ by that their structure and the parameters are determined on the basis of the measurement information by minimization of given criterion (see chapter 3). Two basic groups of such models can be distinguished: the absence of a prior knowledge about structure of a model is characterized for the first one (researcher works it out in result of successive checking of several probable structures); for the second one - structure of a model can be partially or completely determined from the ratio of the material balance or on the basis of pre known descriptions of processes and phenomena. The advantage of the models of the given class is a simplicity and rather low sensitivity to random fluctuations of the researched objects. These models have been fast developed in connection with development of informational - measuring systems with real-time data processing.

In recent years imitative models have been widely applied in solving of many environmental protection problems (see paragraph 3.6). Their advantage implies capabilities of joint application of the first two types of models as interrelated units in general process of imitation. The ability to systematic development and perfection of imitative models in the process of accumulation of new knowledge through advancement separate units or adding new ones makes these models the most perspective ones among all other models of formation

of a state of environmental objects. Besides contrary to the models of the first two classes, imitative models allow to predict multi-version consequences of the future work-loads and strategies of control for the most different environmental objects.

Depending on the available a prior information it is possible to consider different procedures of making decisions (see chapter 4). In the present work, the solution of a certain problem of making decisions is considered. In particular, a problem of testing statistical hypotheses on the condition of environmental object on the basis of results of measurement is considered. With an increase of a prior information it becomes possible to use more complex procedures of testing hypotheses ensuring higher reliability. Therefore in the present work there are brought the different procedures of testing hypotheses depending on the available a prior information and purposes for which they are used.

There are brought mathematical bases of the solution (chapters 1, 2, 3, 4 and 5) and software implementation (chapters 6 and 7) of most important problems of environmental monitoring: mathematical models of pollutants transfer in rivers and identification of sources of emergency pollution of the rivers. The results of investigation of developed software packages are given (see chapters 8).

In the given work the authors aim to systematize the obtained results in the indicated directions during the last years and to set forth them compactly in the most accessible form for a wide range of possible users of the most different specialties and education levels. We would be glad if we managed to reach an objective even partially. All models, methods and algorithms described in the book are realized as software packages for IBM-compatible computers and have the complete off-the shelf packaging for practical application. There are two independent software packages attached to the present book envisaged for the modeling of diffusion of multi-sources water pollutants discharged to rivers and identification of sources of emergency pollutions. These packages are developed in accordance with the world standards of the similar products. Their abilities, user guides, i.e. instructions for input of initial information, making computations and perception of output results, are described in the book (see chapters 6 and 7). We hope that these packages will be the available for researchers, specialists and interested persons for solving problems started before them in respective fields. In case of interest they can address to authors of this book about conditions of acquisition of these packages on the address: kartlos5@yahoo.com.

In conclusion the authors would like to express deep gratitude to the International Science and Technology Center (ISTC) and the U.S. Civilian Research and Development Foundation and its Georgian Branch (CRDF - GRDF), as the majority of results given in this book would not be obtained without financial assistance rendered by these funds within the framework of the project G-047 “Identification of River Water Pollution Sources by Means of Automated Control Systems” and the project GP2-3302 “Development and research of deterministic and stochastic mathematical models for control and management of pollution level of fluvial waters and their realization by application package”.

Chapter 1

DETERMINISTIC MATHEMATICAL MODELS OF POLLUTANTS TRANSFER IN RIVERS

1.1. MATHEMATICAL MODELING OF POLLUTANTS TRANSFER IN RIVERS

Modeling water quality in freshwater ecosystems is considered to be a complex problem due to a high number of factors taking part on the process and the different forms in which pollution can be observed. In this chapter we will focus on water quality models aiming at describing processes of transfer, dilution and self-purification of harmful substances in freshwater ecosystems for rather small interval of time.

Transfer of pollutants is a well know process in general described by the equation of 3D-turbulent diffusion of non-conservative substances [1, 3-5, 25-27, 35]:

$$\begin{aligned}\frac{\partial \Phi}{\partial t} &= \frac{\partial}{\partial x}\left(K_x \frac{\partial \Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial \Phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial \Phi}{\partial z}\right)- \\ &-V_x \frac{\partial \Phi}{\partial x}-V_y \frac{\partial \Phi}{\partial y}-V_z \frac{\partial \Phi}{\partial z}-u\frac{\partial \Phi}{\partial y}-K(\Phi)+f(x,y,z,t),\end{aligned} \tag{1.1}$$

where Φ is the concentration of the non-conservative dissolved substance averaged over time; t is time; x, y, z are the spatial co-ordinates (the axis x is horizontal and its direction coincides with the direction of averaged current of all stream, the axis y is perpendicular to the free surface and it is directed downwards, the axis z is directed across to the stream); K_x, K_y, K_z are the coefficients of the turbulent diffusion in the direction of axes x, y, z; V_x, V_y and V_z are components of speeds on axes x, y, z averaged over time; u represents the largest hydraulic particles; $K(\Phi)$ is the a parameter characterizing the non-conservativeness of pollutant (one often uses simple approximation of this dependence $K(\Phi) \equiv K \cdot \Phi$, where K is the coefficient of non-conservativeness);

$f(x,y,z,t)$ is the total intensity of external sources of pollution. In general, the coefficients K_x, K_y, K_z, V_x, V_y, V_z and $K(\Phi)$ are the functions of a point of space and time [3, 5].

The solution of equation (1.1) concerning the concentration $\Phi(x,y,z,t)$ requires is complex as it depends on sewage discharge conditions, the characteristics of the watercourse, the objective for which the model was developed and the model assumptions made. The combination of the above factors results in different kinds of the equation of three, two or one-dimensional turbulent diffusion equations . The solution of the latest is realized by numerical methods or analytically.

For continuous coastal pollution sources the concentration of the pollutant is known to disseminate non-uniformly on the watercourse. If the non-uniformity of distribution of concentrations of pollutants on the depth of the watercourse is not taken into account, then it is possible to obtain the two-dimensional turbulent diffusion equation [1, 5-7, 12, 28-31] using equation (1.1) as reference:

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \Phi}{\partial y} \right) - V_x \frac{\partial \Phi}{\partial x} - V_y \frac{\partial \Phi}{\partial y} - K\Phi + f. \tag{1.2}$$

Equation (1.2) defines the distribution of concentration of pollutant along and across of the stream taking into account non-uniformity of this distribution. The equation is solved using the method of grids with the transition to the corresponding difference scheme [6-8].

The equation of one-dimensional turbulent diffusion is applied when the distribution of the concentration of the pollutant across the stream is homogeneous. It is also used when average indicators are used to represent pollution across the river. The one-dimensional equation is as follows [5, 9]

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \Phi}{\partial x} \right) - V_x \frac{\partial \Phi}{\partial x} - K\Phi + f(x,t), \tag{1.3}$$

where $f(x,t)$ is a function of a set of pollutants in the watercourse. The one-dimensional equation works under the assumptions that: the concentration of the pollutant is constant across the river, i.e. $\partial\Phi/\partial y = \partial\Phi/\partial z = 0$ and the coefficient of longitudinal turbulent diffusion K_x, the flow and the coefficient of non-conservativeness are constants.

The equation (1.3) is solved for specific initial and boundary conditions, selected in accordance with the type of watercourse. For instantaneous point source of unit mass of pollutant $f(x,t) = \delta(x)\delta(t)/\omega$ is considered an adequate approximation, where ω is the area of living cut. For initial conditions $\Phi(x,0) = 0$ equation (1.3) resolves as follows [10]

$$\Phi(x,t) = \frac{1}{2\omega\sqrt{\pi K_x t}} \exp\left(-\frac{(x - V_x t)^2}{4K_x t} - Kt \right),$$

which justice for the small rivers and channels is proved experimentally [11].

At initial and boundary conditions

$$\Phi(x,0)=\varsigma(x),\quad \Phi(0,t)=f(t),\quad x\in[0,\infty),\quad t\in[0,\infty).$$

Solution of the equation (1.3) looks like [4]

$$\Phi(x,t)=U(x,t)\,e^{\mu x-\lambda t}, \tag{1.4}$$

where

$$\mu=\frac{V}{2a^2};\quad \lambda=\frac{V^2}{4a^2}+K;\quad a^2=K_x;\quad U(x,t)=\omega(x,t)+W_0(x,t);$$

$$W(x,t)=\frac{x}{2a\sqrt{\pi}}\int_0^t\frac{\psi(t-\tau)e^{-\frac{x^2}{4a^2\tau}}}{\tau^{3/2}}d\tau;$$

$$W_0(x,t)=\frac{1}{2a\sqrt{\pi t}}\int_0^\infty\varphi(\theta)[e^{-\frac{(\theta-x)^2}{4a^2t}}-e^{-\frac{(\theta+x)^2}{4a^2t}}]d\theta;$$

$$\varphi(x)=\varsigma(x)e^{-\mu x};\quad \psi(t)=f(t)e^{\lambda t}.$$

In the work [4], special cases of the solution (1.4) are given, when boundary function $f(t)$ is approximated by piecewise linear function or the initial condition is accepted zero.

Solution of the equation (1.3) at initial and boundary conditions

$$\Phi(x,t_0)=\psi(X),\quad \Phi(x_0,t)=\eta(t),\quad f(X,t)=\sum_{i=1}^{k}a_i(t)\,\delta(X-X_i),\quad x_i\in\tau_x,$$

$X\in[x_0,\infty]$, $t>t_0$, i.e. when on water object influence k independent pollution sources, located in spatial points x_i of the considered section of water object J_x with intensities $a_i(t)$ $(i=1,...,k)$, looks like [9]

$$\Phi(X,t_0)=\Phi_1(X,t)+\Phi_2(X,t)+\Phi_3(X,t);$$

$$\Phi_1(X,t)=\sum_{i=1}^{k}\int_{t_0}^{t}g_a(X,x_i,t,\tau)\,a_i(\tau)\,d\tau;$$

$$\Phi_2(X,t)=\int_{t_0}^{t}g_\eta(X,x_0,t,\tau)\,\eta(\tau)\,d\tau;$$

$$\Phi_3(X,t)=\int_{x_0}^{\infty} g_{\psi}(X,x,t,t_0)\,\psi(x)\,dx,$$

where

$g_a(X,x_i,t,\tau)=\frac{1}{2\sqrt{K_x\pi(t-\tau)}}e^{\mu(X-x_i)\lambda(t-\tau)}\left[e^{-\frac{(X-x_i)^2}{4K_x(t-\tau)}}-e^{-\frac{(X+x_i)^2}{4K_x(t-\tau)}}\right]$ is the function of influence of i th source $a_i(t)$;

$g_{\eta}(X,x_0,t,\tau)=\frac{(X-x_0)}{2\sqrt{K_x\pi(t-\tau)^3}}e^{\mu(X-x_0)-\lambda(t-\tau)-\frac{(X-x_0)^2}{4K_x(t-\tau)}}$ is the function of influence of boundary condition $\eta(t)$;

$g_{\psi}(X,x,t,t_0)=\frac{1}{2\sqrt{K_x\pi(t-t_0)}}e^{\mu(X-x)-\lambda(t-t_0)}\left[e^{-\frac{(X-x)^2}{4K_x(t-t_0)}}-e^{-\frac{(X+x)^2}{4K_x(t-t_0)}}\right]$ is the function of influence of initial distribution $\psi(X)$; $\mu=v/2K_x$; $\lambda=K+v^2/4K_x$.

Let us make the comparative analysis of the solutions one- and two-dimensional equations of turbulent diffusion of non-conservative pollutants at constant values of parameters of the stream, coefficients of turbulent diffusion and non-conservativeness [13]. As is shown [4], at piecewise constant approximation of the function $f(t)$, $X=0$ and at the condition of limitation of the function $\Phi(X,t)$ for sufficiently great values X, the equation (1.3) can be solved as follows:

$$\Phi(X,t_m)=\frac{1}{2}\sum_{i=1}^{m-1} f_{i-1}\left[(Q_{m-i+1}-Q_{m-i})+(R_{m-i+1}+R_{m-i})\right], \tag{1.5}$$

where $f_i=f(t_i)$, $t_i=i\cdot\Delta t$, $i=1,...,m$, Δt is the step of splitting of time axis:

$$Q_j=\exp\left(\frac{V-V_0}{2K_x}x\right)\cdot F^*\left(\frac{X-j\Delta tV_0}{2\sqrt{K_x j\Delta t}}\right);$$

$$R_j=\exp\left(\frac{V+V_0}{2K_x}x\right)\cdot F^*\left(\frac{x+j\,\Delta t\,V_0}{2\sqrt{K_x\,j\,\Delta t}}\right); \tag{1.6}$$

$$F^*(z)=1-F(z);\quad F(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-\xi^2}d\xi;$$

$$V_0 = \sqrt{V^2 + 4KK_x}\ . \tag{1.7}$$

For more simple case of constant unit dropping, the expression (1.5) becomes simpler and taking into account (1.6), (1.7), it becomes

$$\Phi_0(X,t) = \frac{1}{2}\left[G(X,t,V_0) + G(X,t,-V_0)\right], \tag{1.8}$$

where

$$G(X,t,\xi) = \exp\left[\frac{V+\varepsilon}{2K_x}x\right]\cdot F^*\left(\frac{x+t\xi}{2\sqrt{K_x t}}\right); \tag{1.9}$$

V_0 is defined by the ratio (1.7).

In works [4, 5] it is specified that the one-dimensional model of turbulent diffusion of non conservative pollutants satisfactorily describes processes of self-purification and transferring pollutants in small streams with small speeds of flow, and solutions obtained on the basis of this model are applicable on the sections located below of some cross-section, called the cross-section of full intermixing. However for solving the majority of considered problems for qualitative estimation of waters, the accuracy of one-dimensional model appears insufficient. In this connection there is a necessity of developing the quantitative estimations which would allow to define borders of action of one-dimensional model of turbulent diffusion depending on the values of the parameters of the stream, characteristics of pollutant and the kind of its dropping. For solving this problem we shall consider the more in detail the equation of two-dimensional turbulent diffusion (1.2).

Let us accept zero initial conditions, i.e. $\Phi(x,y,0) = 0$, at following boundary - conditions:

$$\left.\frac{\partial\Phi}{\partial y}\right|_{y=0,y=H} = 0; \tag{1.10}$$

$$\left.\frac{\partial\Phi}{\partial x}\right|_{x=\infty} = 0, \tag{1.11}$$

where H is the width of a stream. Let us suppose that the pollution source is placed in the beginning of co-ordinates, and the intensity of the drop varies by the law $f(t)$ and weakens on the width of the stream by exponential law, i.e.

$$\Phi(0,y,t)=f(t)\cdot e^{-\beta y},\ \ \beta\ge 0,\ \ 0\le y\le H\ . \tag{1.12}$$

If to introduce dimensionless co-ordinate $\eta=\frac{\pi}{H}y$ and new desired function $U(x,\eta,t)=\Phi(x,\eta,t)\cdot e^{Kt}$, then the system (1.2), (1.10), (1.11) will be transformed to the form

$$\frac{\partial U}{\partial t}=a^2\frac{\partial^2 U}{\partial x^2}+b^2\frac{\partial^2 U}{\partial \eta^2}-V\frac{\partial U}{\partial x},\ \ U(x,\eta,0)=0,\ \ \left.\frac{\partial U}{\partial x}\right|_{x=\infty}=0\ ; \tag{1.13}$$

$$U(0,\eta,t)=f(t)\cdot e^{-\alpha\eta+Kt},\ \ \left.\frac{\partial U}{\partial \eta}\right|_{\eta=0,\pi}=0\ , \tag{1.14}$$

where $a^2=K_x;\ \ b^2=\frac{\pi^2}{H^2}K_y;\ \ \alpha=\frac{H}{\pi}\beta.$

For simplification of the further mathematical calculations, we shall be limited to a case of constant drop of unit intensity, i.e. we shall consider the solution of the system (1.13) at $f(t)=1$. As a result of consecutive application to this system of finite cosine-transformation of Fourier [13] by the variable η

$$F(X,p,t)=F_c\left[U(X,\eta,t)\right]=\int_0^{\pi}U(X,\eta,t)\cos p\eta\, d\eta\ , \tag{1.15}$$

of the substitution

$$\overline{F}=F\cdot\exp(\lambda X+\mu t),$$

where $\lambda=V/(2a^2);\ \ \mu=b^2p^2-V^2/(4a^2)$, and of the Laplace's transformation [14] by the variable t

$$\widetilde{F}(X,p,\xi)=L\left[\overline{F}(X,p,t)\right]=\int_0^{\infty}F(X,p,t)\cdot e^{-\xi\cdot t}dt\ ,$$

we obtain the following system:

$$a^2\frac{\partial^2\widetilde{F}}{\partial x^2}-\xi\overline{F}=0;\ \ \left(\frac{\partial\widetilde{F}}{\partial x}+\lambda F\right)\Big|_{x=\infty}=0;$$

$$F(0,p,\xi)=\frac{1-(-1)^p\cdot e^{-2\pi}}{p^2+\alpha^2}\cdot\frac{\alpha}{\xi-(K-\mu)}.$$

The solution of this system is possible to present in the form

$$\widetilde{F}(x,p,\xi)=\frac{\alpha}{\xi-(K-\mu)}\cdot\frac{1-(-1)^p\cdot e^{-\alpha\pi}}{\alpha^2+p^2}e^{-\frac{\sqrt{\xi}}{\alpha}x}.$$

Applying to this expression consistently inverse transformation of Laplace, the ration - (1.15), inverse transformation of Fourier, and also considering that $\Phi(x,\eta,t)=U(x,\eta,t)\cdot\exp(-Kt)$, and taking into consideration (1.14), the solution (1.2), (1.10), (1.11) is possible to present in the form

$$\Phi(x,y,t)=\frac{1-e^{-\beta H}}{\beta H}\Phi_0(x,t)+\beta H\sum_{p=1}^{\infty}\frac{1-(-1)^p\cdot e^{-\beta H}}{(\beta H)^2+(\pi p)^2}\times$$

$$\times\left[G(x,t,V_p)+G(x,t,-V_p)\right]\cos\left(\frac{\pi}{H}py\right), \qquad (1.16)$$

$$V_p=\sqrt{V^2+4K_x\left[\left(\frac{\pi}{H}p\right)^2+K_y+K\right]}; \qquad (1.17)$$

$\Phi_0(x,t)$ and $G(x,t,\xi)$ are defined by the formula (1.8).

From the condition (1.12) follows that a case when the parameter of dropping $\beta=0$, corresponds to the uniform on width of a stream drop of pollutant. In this connection, the solution (1.16) of the equation of two-dimensional turbulent diffusion coincides with the solution of one-dimensional problem, as $\Phi(x,y,t)\big|_{\beta=0}=\Phi_0(x,t)$, where $\Phi_0(x,t)$ is the solution of one-dimensional equation of turbulent diffusion, defined by the formula (1.8).

The analysis of (1.16) shows that at fixed value of the ratio y/H the increase of the width of a stream H in n time is equivalent to the reduction of the coefficient K_j in n^2 time.

The characteristic form of the function $\Phi(x,y,t)$ in general case, obtained by the formula (1.16) at fixed value of x, is reduced in Fig. 1.1, a.

Detailed analysis of the formula (1.16), realized by means of the computer, has allowed to make following conclusions [12]: 1) the increase of β leads to the increase of heterogeneity of $\Phi(x,y,t)$ in width of a stream, i.e. the value

$$\Delta\Phi = \left[\Phi(x,0,t) - \Phi(x,H,t)\right] / \Phi(x,0,t) \tag{1.18}$$

increases with increasing the value β; 2) the increase of the co-ordinate x, on the contrary, leads to the reduction of $\Delta\Phi$; starting from some value x^*, the value becomes practically equal to 0, i.e. the cross-section, being distant from the place of dropping by the distance x^*, is the cross-section of full mixing; 3) the value x^*, which is the boundary of action of two-dimensional model, depends on the value of the parameter of dropping β, speed V, width H, coefficient K_x and practically does not depend on the coefficient of non-conservativeness q.

For more precise definition of the dependence of x^* on the parameters β, V, H and K_x, the stationary mode of process of distribution of pollutant is considered at unit function of drop, i.e. a case, when $t = \infty$. At this time expressions Φ_0 and Φ, defined by formulas (1.8) and (1.16), become simpler and accept, accordingly, the form

$$\Phi_0 = \Phi(x) = \frac{1}{2} E\left(x, V_0\right); \tag{1.19}$$

$$\Phi = \Phi\left(x, y\right) = \gamma\Phi_0\left(x\right) + \beta H \sum_{p=1}^{\infty} C_p E\left(x, V_p\right) \cos\left(\frac{\pi y}{H} p\right), \tag{1.20}$$

where

$$\gamma = \left[1 - \exp\left(-\beta H\right)\right] / \beta H; \tag{1.21}$$

$$E\left(x, V_p\right) = \exp\left[\frac{\left(V - V_p\right)x}{2K_x}\right]; \tag{1.22}$$

$$C_p = \left[1 - (-1)^p \exp\left(-\beta H\right)\right] / \left[\left(\beta H\right)^2 + \left(\pi p\right)^2\right]; \tag{1.23}$$

V_p is defined by the ratio (1.17), $p = 0,1,2,3,\ldots$ The Characteristic form of the function $\Phi\left(x, y\right)$, defined by the formula (1.20), is presented in Fig. 1.1, b.

The value x^* was defined as minimum value of the co-ordinate x, starting from which the relative error $\Delta\Phi$ (1.18) will not exceed 5 %:

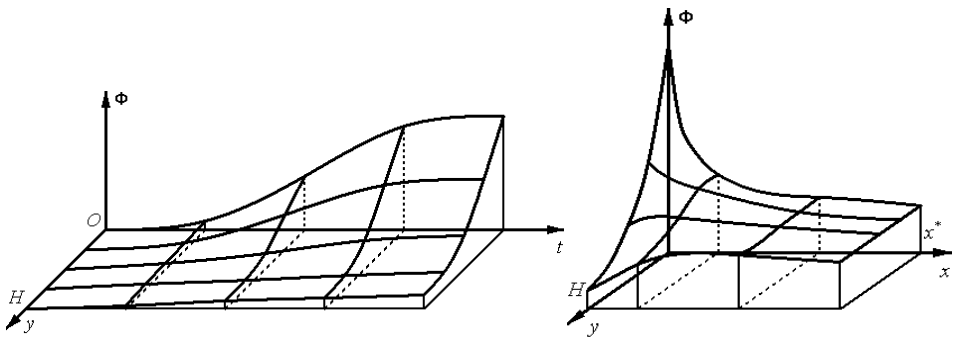
$$\left[\Phi(x,0)-\Phi(x,H)\right]/\Phi(x,0)<0{,}05\,, \tag{1.24}$$

where $\Phi(x,0)$ and $\Phi(x,H)$ were defined according to (1.20) by ratios

$$\Phi(x,0)=\gamma\,\Phi_0+\beta\,H\sum_{p=1}^{\infty}C_p\,E(x,V_p)\,;$$

$$\Phi(x,H)=\gamma\,\Phi_0+\beta\,H\sum_{p=1}^{\infty}(-1)^p\,C_p\,E(x,V_p)\,;$$

Φ_0 – by the formula (1.19), and, and γ, E and C_p – by (1.21) – (1.23).



a b

Figure 1.1. Graphic representation of the concentration $\Phi=\Phi(x,y,t)$ at fixed value of longitudinal co-ordinate x (a) and in stabilized mode $t=0$ (b).

The condition (1.24), used for finding x^*, is possible to present in the form

$$39\,\sigma_1-\sigma_2<\gamma\,\Phi_0\,, \tag{1.25}$$

where $\sigma_1=\beta\,H\sum_{l=1}^{\infty}C_{2l-1}\,E(x,V_{2l-1})$; $\sigma_2=\beta\,H\sum_{l=1}^{\infty}C_{2l}\,E(x,V_{2l})$.

The analysis of values x^* (km), obtained by means of the computer from the condition (1.25) at various values of parameters V (km/h), K_x (km^2/h), H (km) and β, has allowed to establish the following dependence:

$$x^*=\varphi(K_x)\,V\,\widetilde{H}^2\left(1-e^{-\beta H}\right), \tag{1.26}$$

where $\varphi(K_x)$ represents the function, close to linear concerning the variable K_x; $\widetilde{H}$ is the resulted value of the width of the stream, defined by the ratio $\widetilde{H} = \dfrac{0{,}06}{\sqrt{K_y}} H$.

Linearization of the function $\varphi(K_x)$ has allowed to present the formula (1.26) for finding the border of action of two-dimensional model in the form [12]

$$x^* = (1{,}55\, K_x + 0{,}44)\, VH^2 \frac{1}{K_y}\left[1 - \exp\left(-\beta \frac{0{,}06}{\sqrt{H_y}} H\right)\right]. \tag{1.27}$$

In cases when drop of pollutant is sharply concentrated on width, i.e. β is great enough, for finding x^*, the use of more simple formula is possible:

$$x^* \approx 0{,}45\, V \frac{1}{K_y} H^2 . \tag{1.28}$$

This formula can be used for obtaining the upper estimation of the value x^* in cases when the value β is not known. In cases when sewage cause essential increase in the discharge of water in the stream of water, for taking into account of unsteady movement of the stream by calculation of its hydraulic characteristics the equation of Saint-Venant is used [7, 15]:

$$W \frac{\partial z}{\partial t} + \frac{\partial Q}{\partial x} = \upsilon; \quad \frac{\partial Q}{\partial t} + \frac{\partial (VQ)}{\partial x} = \upsilon\omega\left(\frac{\partial z}{\partial x} + \frac{Q|Q|}{K^2}\right), \tag{1.29}$$

where W is the width of the surface of the water; z is a mark of free surface; Q is the discharge of the water; V is the speed of the flow; υ is intensity of lateral inflow of the water; ω is the area of live section of the river-bed; K is the module of the expense, $K = \omega \hat{C}\sqrt{R}$; C is the coefficient of Shezy; R is hydraulic radius. The problem (1.29), as well as (1.1), (1.2), solves by numerical methods, in particular, by the method of grids [8, 16].

In works [15, 17, 18], the multi-component models, considering transformation of one pollutant in another (for example, consecutive transformation of compounds of nitrogen), are considered; they are based on the equations of balance of pollutant and the equations of hydraulics of flows with corresponding initial and boundary conditions. Diffusion coefficients, speed of the flow of a stream, the characteristic of streams were supposed known in these models, which in a real situation are defined from hydraulic calculations on the basis of natural observations. Besides, in models the errors of measurement, essentially influencing results of calculations, were not considered. If the size of the measuring information is

significant (in the sense of mathematical statistics), then instead of similar enough difficult models much more effectively is to pass to more simple statistical models which, at the same time, are steadier against errors of measurements [1, 3, 19, 20]. Such models are considered in Chapter 3 of the present monograph.

In work [21], models of eftrofication for modeling of seasonal change of concentration of sea seaweed depending on the use of fertilizers are given. These models were used for computer realization of the methodology developed in works [23, 24], and also for carrying out of numerical experiment. In work [22], the further development of these models in the form of three-dimensional eftroficating numerical model is given. The last, along with the quality of the water, describes also hydrodynamics and simultaneously unites requirement of oxygen and isolation of nutrients from sediments.

In work [25], questions of hydrochemistry, hydrodynamics and hydrobiology, connected with so-called intra-reservoir processes are considered. The analysis of modern methods of studying the basic intra-reservoir processes is given and the necessity of the development of the methodology, methods and means of natural modeling of hydrodynamic and chemical-biological processes is shown.

In work [32], many processes proceeding in the environment which are solved by means of modeling, including processes of pollution and processing of sewage are described. Both in the book and on enclosed diskette many examples of modeling are resulted. They are realized in the language of modeling ISIM and are ready to use for carrying out of calculations on the computer in operational system DOS. This possibility will allow the reader to penetrate into the essence of mathematical models and modeling process more deeply.

In the collective monograph [32], the problem of quality of water is considered from the uniform system point of view. In the first part of the book, the technique of the system analysis which includes not only the use of this or that mathematical apparatus, but also the basic concepts of their application is studied. The second part of the book contains examples of application of the offered methods to the solution of concrete tasks of different level. Those are: models of primary production in fresh-water reservoirs, models of nitrification process in real river system, models of transferring pollutants in the estuaries and open sea. The set of practical examples is given in the book.

In the monograph [34], the deterministic-probability approach to the description and forecasting of polluting processes of superficial waters by using hardware-software means of mathematical modeling is offered; it includes: the method of electro-convective-diffusion analogy and its realization on analogue computers and on the hybrid computer complex; complex factor-cluster-taxonomy method and its realization on the computer; package of applied programs for the forecast of the field of concentration and computation of maximum permissible drop on the computer.

In [41] are considered one-dimensional Saint-Venant classical equations and numerical algorithms for describing the processes of heat and mass transfer in river flows, the sedimentation and stirring-up of pollutants taken into account. Some results of numerical experiments are given.

In [228] is presented a simple mathematical model for river pollution and is investigated the effect of aeration on the degradation of pollutant. The model consists of a pair of coupled reaction-diffusion-advection equations for the pollutant and dissolved oxygen concentrations, respectively. The coupling of these equations occurs because of reactions between oxygen and pollutant to produce harmless compound. There is considered the steady-state case in one

spatial dimension. For simplified cases the model is solved analytically. Also is presented a numerical approach to the solution in the general case. There is shown that for the Tha Chin River in Thailand simple models can provide decision support for planning restrictions to be imposed on farming and urban practices.

1.2. MATHEMATICAL MODELS OF TRANSFER AND TURBULENT DIFFUSION

Dynamics of transfer of pollutants in river water is described by the diffusion equations. Usually these equations should be solved numerically, with the help of difference schemes. Here are some questions, related to the choice of methods of solving various problems from which the practical realizability, the accuracy and the duration of obtaining the solution on the computer depend on. In particular: a) the analytical description of flat or spatial area for which the equations of diffusion and boundary conditions are investigated, i.e. the analytical - description of coastal lines and a river bed; b) the analytical description of the dependence of coefficients of the equation from spatial co-ordinates; c) the analytical description of dependence on spatial co-ordinates and from time of non-uniform parts of the solved equations of diffusion, i.e. powers of pollution sources; d) the correct choice in difference scheme ratios between spatial steps of the grid, and also between them and the step of digitization of time.

The listed questions are considered by authors of the presented work in [36–40]. The basic results are given below after formulation of the problem of dissemination of pollutants in the form of equation of transfer and diffusion with additional conditions, and review of known numerical methods of solving these equations.

For clearness we shall introduce the following designations, used in future.

Parameters defining geometry and dynamics of the considered section of the river: x, y – horizontal Descartes co-ordinates (m); ξ – longitudinal co-ordinate (m); η – transverse co-ordinate (m); z – vertical Descartes co-ordinate (m); t – parameter of time (sec); $W(x)$ – the width of the river (m); $E(x)$ – the area of cross-section of the river (m^2); $H(x, y)$ – the depth of the river (m); $v(r)$ – the velocity of the flow (m/sec).

Parametres of river water: s, S, σ – the concentration of the pollutant (mg/m^3); $f(t,r)$ – power of pollution sources (mg/m^3); $F_j(t)$ – integrated power of j th pollution source (mg/sec); $p_j(t)$ – the discharge of water by j th source of pollution (m^3/sec); $K(r)$ – tensore of turbulent diffusion (m^2/sec); $\zeta(r)$ – coefficient of non conservativeness (sec^{-1}); q – coefficient of self-purification; l – the length of self-purification (m).

Each of water parameters corresponds to some pollutant from the list of polluting components by which modeling is realized. By M we shall designate the number of pollutants from the available list, common for all sections, and by R – the number of sources of pollution from the list, corresponding to the considered section. The index j is the number of the source of pollution operating on the considered –section of the river.

For calculation of the power of sources of pollution we shall use the following formula:

$$f(t,r)=\sum_{j=1}^{R}F_j(t)\cdot\delta(r-r_j);\quad F_j(t)=p_j(t)\cdot S_j(t),$$

where $S_j(t)$ is the concentration of the pollutant dropped by j th source of pollution in the water; r_j is the radius-vector of the action of this source.

1. Possible types of models. The concentration of the pollutant transferred in river water is defined by the formula

$$s=\Phi(t,r)\cdot P_0/P, \tag{1.30}$$

where $\Phi(t,r)$ is the solution of one of brought below diffusion equations; P is the discharge of water in a current point; P_0 is the discharge of water in upper section of considered section, i.e. at $x=0$.

Investigated equation is m-dimensional equation of diffusion. We shall consider following models: 1) one-dimensional model ($m=1$); 2) two-dimensional model ($m=2$); 3) three-dimensional model ($m=3$). Three-dimensional model is the most exact among considered. Other models should be considered as special cases of three-dimensional model. Concerning their practical use depending on characteristics of the rivers and solved problems see paragraph 8.4.

In one-dimensional model instead of tensor of turbulent diffusion $K(r)$, one of its component – the coefficient of turbulent diffusion $K(x)=K_{xx}(r)$, is used only. In two-dimensional and three-dimensional models tensor $K(r)$ is supposed diagonal.

In given below two-dimensional and three-dimensional equations of diffusion independent variables are t, x, y, z. Here the given equations have the traditional form of record in which it is supposed that the considered section of the river lasts along the axis of abscess, not deviating aside. If the river on the considered section is twisting then in the equations horizontal Cartesian co-ordinates x and y should be replaced by appropriate - curvilinear – longitudinal and transverse co-ordinates ξ and η. Definition of these co-ordinates and their relation to the Cartesian co-ordinates are described in paragraph 1.4.1.

2. The equation of diffusion for one-dimensional model. The equation looks like

$$E(x)\cdot\frac{\partial}{\partial t}\Phi(t,x)-\frac{\partial}{\partial x}\left(E(x)\,K(x)\cdot\frac{\partial}{\partial x}\Phi(t,x)\right)+$$
$$+E(x)\,v(x)\cdot\frac{\partial}{\partial x}\Phi(t,x)+E(x)\,\zeta(x)\cdot\Phi(t,x)=E(x)\,f(t,x), \tag{1.31}$$

where

$$E(x)\, f(t,x) = \sum_{j=1}^{R} F_j(t) \cdot \delta(x - x_j) \quad . \tag{1.32}$$

3. The equation of diffusion for two-dimensional model. The equation looks like

$$H(r) \cdot \frac{\partial}{\partial t}\Phi(t,r) - \frac{\partial}{\partial x}\left(H(r)\, K_{xx}(r) \cdot \frac{\partial}{\partial x}\Phi(t,r) \right) -$$
$$- \frac{\partial}{\partial y}\left(H(r) K_{yy}(r) \cdot \frac{\partial}{\partial y}\Phi(t,r) \right) + H(r)\left(v_x(r) \cdot \frac{\partial}{\partial x}\Phi(t,r) + v_y(r) \cdot \frac{\partial}{\partial y}\Phi(t,r) \right) +$$
$$+ H(r)\, \zeta(r) \cdot \Phi(t,r) = H(r)\, f(t,r),$$

or in vectorial form

$$H(r) \cdot \frac{\partial}{\partial t}\Phi(t,r) - \left(\nabla \cdot \left(H(r)\, K(r)\right) \cdot \nabla\right) \cdot \Phi(t,r) +$$
$$+ H(r)\left(v(r) \cdot \nabla\right) \cdot \Phi(t,r) + H(r)\, \zeta(r) \cdot \Phi(t,r) = f(t,r), \tag{1.33}$$

where $r = [x, y]$;

$$H(r)\, f(t,r) = \sum_{j=1}^{R} F_j(t) \cdot \delta(x - x_j)\delta\left(y - y_j\right). \tag{1.34}$$

4. The equation of diffusion for three-dimensional model. The equation looks like

$$\frac{\partial}{\partial t}\Phi(t,r) - \sum_{l=1}^{3} \frac{\partial}{\partial r_l}\left(K_{ll}(r) \cdot \frac{\partial}{\partial r_l}\Phi(t,r) \right) +$$
$$+ \sum_{l=1}^{3} v_l(r) \cdot \frac{\partial}{\partial r_l}\Phi(t,r) + \zeta(r) \cdot \Phi(t,r) = f(t,r),$$

or in vectorial form

$$\frac{\partial}{\partial t}\Phi(t,r) - \left(\nabla \cdot K(r) \cdot \nabla\right) \cdot \Phi(t,r) + \left(v(r) \cdot \nabla\right) \cdot \Phi(t,r) + \zeta(r) \cdot \Phi(t,r) = f(t,r), \tag{1.35}$$

where $r = [r_1, r_2, r_3] = [x, y, z]$;

$$f(t,r) = \sum_{j=1}^{R} F_j(t) \cdot \delta(x - x_j)\delta\left(y - y_j\right)\delta\left(z - z_j\right) \quad . \tag{1.36}$$

5. Domain of definition of the equation of diffusion. The function $\Phi(t,r)$ is considered defined at $t \geq 0$ and $r \in G$, where G is one-dimensional interval, flat or spatial area, for which the diffusion equation is solved. This area is set by means of inequalities:

$0 \leq x \leq \Im$;

$\eta_r(x) \leq y \leq \eta_l(x) \quad (m \geq 2)$;

$0 \leq z \leq H(x,y) \quad (m = 3)$;

where $\eta_r(x)$, $\eta_l(x)$ and $H(x,y)$ are given functions. At use of classical boundary conditions $\Im = 2L$; otherwise $\Im = L + l$ (L is the length of considered section of the river). Functions $\eta_r(x)$ and $\eta_l(x)$ define position on horizontal plane, accordingly, the right and left coast of the river. The function $H(x,y)$ defines the position of river bed in space, i.e. defines values of the depth of the river in various points.

Thus, the border of the area G, which we shall designate by ∂G, is possible to divide - into some parts. Among them – the upper and the lower cross-sections of the river, in which, $x = 0$ and $x = \Im$, respectively; in one-dimensional model this is simply points which are the ends of the interval G. At $m = 2$ the border ∂G contains also river coasts, and at $m = 3$ – lateral walls (if they are available), river bed and upper free surface.

6. Initial and boundary conditions of solving the equation of diffusion. Additional conditions are set in the form

$$\Phi(0,r) = S_0; \quad \Phi(t,r)\big|_{x=0} = \sigma$$

($S_0, \sigma = const$). Boundary conditions in the lower end of the section can be classical or non-classical. Classical condition looks like

$$\frac{\partial}{\partial x}\Phi(t,r)\big|_{x=\Im} = 0 \text{; (condition of full mixing)} \tag{1.37}$$

non-classical condition –

$$\Phi(t,r)\big|_{x=\Im} = q \cdot \Phi(t,r)\big|_{x=\Im-l} \text{. (not local boundary condition)} \tag{1.38}$$

where q is the coefficient of self-purification of the river on the considered section; ω is the concentration of the pollutant dropped by pollution source in the point $x = \Im$ [30, 42, 224].

At $m \geq 2$, boundary conditions on the other part of the line or on the surface ∂G – Neumann's conditions, are set also

$$(\nu \cdot \nabla)\, \Phi(t,r)\big|_{r\in\partial G} = 0, \tag{1.39}$$

where ν is unit vector of external normal to the border ∂G. In particular, at $m = 3$, it should be

$$\frac{\partial}{\partial z}\Phi(t,r)\Big|_{z=0} = 0. \tag{1.40}$$

1.3. SOME ANALYTICAL METHODS USING AT SOLVING MULTIDIMENSIONAL PROBLEMS

At modeling, before and after numerical solution of the equations of diffusion, often there is expedient to apply, to these equations and their solutions, some analytical methods for simplification of algorithms of solution, for evidence and clearness of obtained results. Some of these methods are considered in the present paragraph.

1. Replacement of variables in the diffusion equation. Let us consider m-dimensional ($m \geq 1$) equation of diffusion

$$D(t,x)\cdot\frac{\partial}{\partial t}\Phi(t,x) + \left(-\left(\nabla\cdot\mathbf{A}(x)\cdot\nabla\right) + \left(\boldsymbol{B}(x)\cdot\nabla\right) + C(x)\right)\cdot\Phi(t,x) = f(t,x),$$

which is required to be solved for some area G of m-dimensional space taking into account the set of initial and boundary conditions.

For using the algorithm described in paragraph 2.1 at solving the given equation, it is necessary, first of all, by replacement of independent spatial co-ordinates, to transform the area G in the hyper-parallelepiped which co-ordinates of points satisfy inequalities

$$a_k \leq x_k \leq b_k \quad (k = 1,...,m).$$

Let the replacement of variables by formulae

$$\widetilde{x}_k = \varphi_k(x_1,...,x_m) \quad (k = 1,...,m)$$

leads to the required transformation of the area G. At such replacement the considered differential equation will be transformed to the similar equation

$$\widetilde{D}(t,\widetilde{x})\cdot\frac{\partial}{\partial t}\widetilde{\Phi}(t,\widetilde{x})+\left(-\left(\widetilde{\nabla}\cdot\widetilde{\mathbf{A}}(\widetilde{x})\cdot\widetilde{\nabla}\right)+\left(\widetilde{\boldsymbol{B}}(\widetilde{x})\cdot\widetilde{\nabla}\right)+\widetilde{C}(\widetilde{x})\right)\cdot\widetilde{\Phi}(t,\widetilde{x})=\widetilde{f}(t,\widetilde{x}),$$

where

$$\widetilde{\nabla}_k\equiv\partial/\partial\widetilde{x}_k\quad(k=1,...,m);$$

$$\widetilde{\Phi}(t,\widetilde{x})=\Phi(t,x);\quad\widetilde{f}(t,\widetilde{x})=f(t,x);$$

$$\widetilde{D}(t,\widetilde{x})=D(t,x);\quad\widetilde{C}(t,\widetilde{x})=C(t,x);$$

In the new equation coefficients $A_{jk}(x)$ and $B_k(x)$ are replaced, accordingly, by coefficients $\widetilde{A}_{jk}(\widetilde{x})$ and $\widetilde{B}_k(\widetilde{x})$, expressions of which, in general case, are very bulky; at this time, if the matrix $\mathbf{A}(x)$, appearing in the initial equation, is diagonal, the matrix $\widetilde{\mathbf{A}}(\widetilde{x})$, appearing in the transformed equation, generally speaking, is not diagonal.

However at calculation of the concentration of pollutants we will consider a case when the surface, limiting the area G, is enough smooth (in particular, river coast should be cut poorly up). At this time, functions $\varphi_k(x)$ $(k=1,...,m)$ can be chosen so that in obtained, after replacement of variables, diffusion equation it was possible to neglect coefficients at mixed derivatives. In other words, at a suitable choice of new variables, it is possible to consider the matrix $\widetilde{\mathbf{A}}(\widetilde{x})$ diagonal.

2. Replacement of variables in two-dimensional equation of diffusion. Let us consider the equation of diffusion given in the previous Item, at $m=2$; the vector composed by spatial co-ordinates, here we will designate by $r=[x,y]$. If, according to conditions of Item 5 of the paragraph 1.2, the domain of change of the variables x and y is defined by conditions

$$0\le x\le\Im;\quad\eta_r(x)\le y\le\eta_l(x),$$

then replacement of variables by formulae

$$\widetilde{x}=x;\quad\widetilde{y}=\frac{W_0\cdot\left(y-\eta_r(x)\right)}{\eta_l(x)-\eta_r(x)};$$

where $W_0=const$, leads to the required transformation of the domain G: the domain of change of the variables $\widetilde{x}$ and $\widetilde{y}$ is the rectangle

$$0 \le \widetilde{x} \le \Im; \quad 0 \le \widetilde{y} \le W_0.$$

The constant W_0 can be any, but is expedient to accept it equal to the average width of the river on the considered section.

If the tensor $\mathbf{A}(x)$ is diagonal and if in the expressions, defining coefficients of the transformed equation of diffusion, to neglect the first and second derivatives of the functions $\eta_l(x)$, $\eta_r(x)$ by x, then we shall obtain the following expressions for new coefficients:

$$\widetilde{A}_{xy}(\widetilde{r}) = 0;$$

$$\widetilde{A}_{xx}(\widetilde{r}) = A_{xx}(r); \quad \widetilde{A}_{yy}(\widetilde{r}) = \frac{W_0^2 \, A_{yy}(r)}{(\eta_l(x) - \eta_r(x))^2};$$

$$\widetilde{B}_x(\widetilde{r}) = B_x(r); \quad \widetilde{B}_y(\widetilde{r}) = \frac{W_0^2 \, B_y(r)}{\eta_l(x) - \eta_r(x)}.$$

3. Replacement of variables in three-dimensional equation of diffusion. Let us consider the equation of diffusion given in Item 1, at $m = 3$. The vector composed by spatial co-ordinates, here we shall designate by $r = [x, y, z]$. If, according to conditions of Item 5 of the paragraph 1.2, the domain of change of variables x, y, z, is defined by conditions

$$0 \le \widetilde{x} \le \Im; \quad \eta_r(x) \le y \le \eta_l(x); \quad 0 \le z \le H(x, y),$$

then replacement of variables by formulae

$$\widetilde{x} = x; \quad \widetilde{y} = \frac{W_0 \cdot (y - \eta_r(x))}{\eta_l(x) - \eta_r(x)}; \quad \widetilde{z} = \frac{H_0 \cdot z}{H(x, y)},$$

where $W_0, H_0 = const$, leads to required transformation of the domain G: the domain of change of variables $\widetilde{x}$, $\widetilde{y}$, $\widetilde{z}$, is the parallelepiped

$$0 \le \widetilde{x} \le \Im;$$
$$0 \le \widetilde{y} \le W_0; \quad 0 \le \widetilde{z} \le H_0.$$

Constants W_0 and H_0 can be any, but it is expedient to accept them equal to the average width and the average depth of the river on the considered section.

If the tensor $\mathbf{A}(x)$ is diagonal and if in the expressions, defining coefficients of the transformed equation of diffusion, to neglect the first and second derivatives of functions

$\eta_l(x)$, $\eta_r(x)$ by x and functions by x and y, then we shall obtain the following expressions for new coefficients:

$$\widetilde{A}_{xy}(\widetilde{r}) = \widetilde{A}_{yz}(\widetilde{r}) = \widetilde{A}_{zx}(\widetilde{r}) = 0;$$

$$\widetilde{A}_{xx}(\widetilde{r}) = A_{xx}(r); \quad \widetilde{A}_{yy}(\widetilde{r}) = \frac{W_0^2\, A_{yy}(r)}{(\eta_l(x) - \eta_r(x))^2}; \quad \widetilde{A}_{zz}(\widetilde{r}) = \frac{H_0^2\, A_{zz}(r)}{(H(x,y))^2};$$

$$\widetilde{B}_x(\widetilde{r}) = B_x(r); \quad \widetilde{B}_y(\widetilde{r}) = \frac{W_0^2\, B_y(r)}{\eta_l(x) - \eta_r(x)}; \quad \widetilde{B}_z(\widetilde{r}) = \frac{H_0^2\, B_z(r)}{H(x,y)}.$$

4. Using of the principle of super-position. Let for definition of the concentration of the considered pollutant, the model is used in which this concentration $s = \Phi(t,r)$ is the solution of one of the equations of diffusion given in the paragraph 1.2 with non-uniform part

$$D(t,r)\, f(t,r) = \sum_{j=1}^{R} F_j \cdot \delta(r - r_j),$$

($F_j = const$) with initial and boundary conditions

$$\Phi(0,r) = \sigma; \qquad \Phi(t,r)\big|_{x=0} = \sigma$$

($\sigma = const$) and

$$(\nu \cdot \nabla)\Phi(t,r) = 0$$

on other part of the border of considered spatial area for which ν is unit vector of external normal. In this model on the considered section of the river function R dot sources of pollution; power of j th source $F_j = p_j S_j$ ($j = 1,...,R$), where the discharge of water p_j and the concentration of the pollutant in this water S_j are considered not to be dependent on time.

Sometimes (for example, at detection of emergency pollution sources of the river (see Chapters 5, 7)), in order to economy of time and memory of the computer, it is required to make preliminary calculation of the concentration of pollutants in the rivers for different modes of drops from pollution sources, acting on the given section of the river. The results of the calculation will be repeatedly used further. In such cases, it is convenient to present required concentration in the form

$$s = \sigma \cdot u_0 + \sum_{j=1}^{R} F_j \cdot u_j ,$$

where u_0 is the solution of the considered diffusion equation in which the non-uniform part is rejected, with initial and boundary conditions

$$\Phi(0,r) = 1, \quad \Phi(t,r)\big|_{x=0} = 1 ;$$

For each value of j, u_j is the solution of the considered equation of diffusion with zero initial and boundary (at $x = 0$) conditions in which the non-uniform part is replaced by function $\delta(r - r_j)$.

5. Rough estimate of the result. Let for definition of the concentration of considered pollutant the same model serves about which it was spoken in the previous Item. At $t > t_j$ for all values j, where t_j is time during which the pollutant is transferred by the flow from j th source to the point of supervision, as a rough estimate of desired concentration can serve the number

$$s_0 = \frac{P_0 \cdot \sigma + \sum_{j=1}^{R} p_j S_j}{P_0 + \sum_{j=1}^{R} p_j} ,$$

where P_0 is the water discharge in the upper end of the section. Such approach means that the concentration of considered pollutant is considered homogeneous, i.e. uniformly distributed on all cross-section and on all length from sources up to the place of supervision.

If to use the given approach and if to consider that the discharges of the water which are poured in the river by each pollution source, is much less than water discharge in the river, i.e. $p_j << P_0$, then auxiliary solutions of the considered equation of diffusion, about which was spoken in the previous Item, can be defined as follows:

$$u_0 \approx 1; \quad u_j \approx 1 / P_0 .$$

In future the value s_0 we shall call the average concentration. Results of the numerical solution of the equation of diffusion can be compared to it.

In following two Items the generalization of known, often used method of linear - interpolation of the function of one real variable for the case, when the function of two or

three variables is considered, is given. The given formulae are used in the computer - packages, described in Chapters 6 and 7, for visual representation of solutions of the two- and three-dimensional equations of diffusion, obtained by numerical methods.

6. Linear interpolation of the function of two variables. Let the function $u = f(x, y)$ is given in the rectangular area defined by inequalities $A_x \le x \le B_x$; $A_y \le y \le B_y$, in the form of the table, where x_j, y_k, u_{jk} ($j = 0,..., N_x; k = 0,..., N_y$) are elements of given numerical sequences. Let us designate for fixed j and k

$$x_a = x_j; \quad x_b = x_{j+1}; \quad y_a = y_k; \quad y_b = y_{k+1};$$

$$u_{aa} = u_{jk}; \quad u_{ab} = u_{j,k+1}; \quad u_{ba} = u_{j+1,k}; \quad u_{bb} = u_{j+1,k+1}.$$

Linear interpolation is consisted in the following that in the rectangle $x_a \le x \le x_b$; $y_a \le y \le y_b$, the function $f(x, y)$ is approximated by the function $S_{jk}(x, y)$, which is linear in relation to any of variables x, y at fixed value of other variable:

$$S_{jk}(x, y) = \frac{p_0 + p_1 x + p_2 y + p_{12} xy}{(x_b - x_a)(y_b - y_a)},$$

where

$$p_0 = x_b y_b u_{aa} - x_b y_a u_{ab} - x_a y_b u_{ba} + x_a y_a u_{bb};$$
$$p_1 = -y_b u_{aa} + y_a u_{ab} + y_b u_{ba} - y_a u_{bb};$$
$$p_2 = -x_b u_{aa} + x_b u_{ab} + x_a u_{ba} - x_a u_{bb};$$
$$p_{12} = u_{aa} - u_{ab} - u_{ba} + u_{bb}.$$

7. Linear interpolation of the function of three variables. Let the function $u = f(x, y, z)$ is given in the parallelepiped, defined by inequalities $A_x \le x \le B_x$; $A_y \le y \le B_y$; $A_z \le z \le B_z$, in the form of the table $u_{jkl} = f(x_j, y_k, z_l)$, where x_j, y_k, z_l, u_{jkl} ($j = 0,..., N_x; k = 0,..., N_y; l = 0,..., N_z$) are elements of the given numerical sequences. Let us designate for fixed j, k and l

$$x_a = x_j; \quad x_b = x_{j+1}; \quad y_a = y_k; \quad y_b = y_{k+1}; \quad z_a = z_l; \quad z_b = z_{l+1};$$

$u_{aaa} = u_{jkl}$; $u_{aab} = u_{j,k,l+1}$;

$u_{aba} = u_{j,k+1,l}$; $u_{abb} = u_{j,k+1,l+1}$;

$u_{baa} = u_{j+1,k,l}$; $u_{bab} = u_{j+1,k,l+1}$;

$u_{bba} = u_{j+1,k+1,l}$; $u_{bbb} = u_{j+1,k+1,l+1}$.

Linear interpolation is consisted in the following that in the parallelepiped $x_a \le x \le x_b$; $y_a \le y \le y_b$; $z_a \le z \le z_b$, the function $f(x,y,z)$ is approximated by the function $S_{jkl}(x,y,z)$, which is linear in relation to any of variables x, y, z at fixed values of other variables:

$$S_{jkl}(x,y,z) = \frac{p_0 + p_1 x + p_2 y + p_3 z + p_{12} xy + p_{23} yz + p_{31} zx + p_{123} xyz}{(x_b - x_a)(y_b - y_a)(z_b - z_a)},$$

where

$$p_0 = x_b y_b z_b u_{aaa} - x_b y_b z_a u_{aab} - x_b y_a z_b u_{aba} + x_b y_a z_a u_{abb} -$$
$$- x_a y_b z_b u_{baa} + x_a y_b z_a u_{bab} + x_a y_a z_b u_{bba} - x_a y_a z_a u_{bbb};$$
$$p_1 = y_b z_b (u_{baa} - u_{aaa}) + y_b z_a (u_{aab} - u_{bab}) + y_a z_b (u_{aba} - u_{bba}) + y_a z_a (u_{bbb} - u_{abb});$$
$$p_2 = x_b z_b (u_{aba} - u_{aaa}) + x_b z_a (u_{aab} - u_{abb}) + x_a z_b (u_{baa} - u_{bba}) + x_a z_a (u_{bbb} - u_{bab});$$
$$p_3 = x_b y_b (u_{aab} - u_{aaa}) + x_b y_a (u_{aba} - u_{abb}) + x_a y_b (u_{baa} - u_{bab}) + x_a y_a (u_{bbb} - u_{bba});$$
$$p_{12} = z_b (u_{aaa} + u_{bba} - u_{aba} - u_{baa}) + z_a (u_{abb} + u_{bab} - u_{aab} - u_{bbb});$$
$$p_{23} = x_b (u_{aaa} + u_{abb} - u_{aab} - u_{aba}) + x_a (u_{bab} + u_{bba} - u_{baa} - u_{bbb});$$
$$p_{31} = y_b (u_{aaa} + u_{bab} - u_{aab} - u_{baa}) + y_a (u_{abb} + u_{bba} - u_{aba} - u_{bbb});$$
$$p_{123} = u_{aab} - u_{aaa} - u_{abb} + u_{aba} - u_{bab} + u_{baa} + u_{bbb} - u_{bba}).$$

1.4. DESCRIPTION OF RIVER BANKS BY SPLINES

The question of analytical setting plane or spatial areas, for which the diffusion equation and boundary conditions are investigated, is considered [37]. This area is the part of the bed of the river on the considered section, filled by water.

There is introduced the system of orthogonal curvilinear coordinates which serve for simplification analytical description of plane area, restricted by coastal lines of the river. Such

description is necessary for numerical solution of diffusion equation, describing the change of concentrations of pollutants in river water.

For analytical description of plane curve, given in the form of the sequence of not coinciding points with certain Cartesian coordinates, which, in particular, can be one of the coastal lines of the river, the interpolation by splines is used. Algorithms of construction of two splines, having explicit forms and provided continuous dependence of tangential vector of the curve from its parameter, are described.

1.4.1. The Contour of the River

For analytical setting of the bank lines, in order to simplify the calculations, it is expedient to use curvilinear coordinates instead of Cartesian coordinates, which are connected with some conditional curve, which stretches along the river between its banks. Hereinafter this curve we shall call *contour of the river*. This expediency is conditioned by two facts given below: the first is the relation of one of the Cartesian coordinates of points of the bank lines from other coordinate can be multiple valuted in connection with a veering of the river, while the lines can be specified in the explicit form in curvilinear coordinates if the river contour is selected properly and its banks are not hardly indented. Secondly, under certain conditions [5] the diffusion equations in curvilinear coordinates do not contain mixed derivative and, therefore, the problem of their numerical solution is essentially simplified.

Suppose some curve is given in the parametric form

$$x = \varphi_1(\xi); \quad y = \varphi_2(\xi),$$

where ξ is the length of the curve beginning from some point; i.e.

$$(\dot{\varphi}_1(\xi))^2 + (\dot{\varphi}_2(\xi))^2 = 1, \tag{1.41}$$

takes place, where the dots over the functions mean their derivatives.

It is possible to specify orthogonal curvilinear coordinates ξ, η, by which Cartesian coordinates x, y can be expressed by the following formulas:

$$\begin{aligned} x &= \varphi_1(\xi) - \dot{\varphi}_2(\xi) \cdot \eta; \\ y &= \varphi_2(\xi) + \dot{\varphi}_1(\xi) \cdot \eta. \end{aligned} \tag{1.42}$$

The coordinates ξ and η have a simple geometrical sense: the point $P_{\xi\eta}$ with given coordinates lies on the normal to the curve passing through its point $P_{\xi 0}$, corresponding to the value of the parameter equal to ξ, and apart from the point $P_{\xi 0}$ on the distance $|\eta|$, and

$P_{\xi\eta}$ is to the left of tangent vector to the curve in the point $P_{\xi 0}$ at $\eta > 0$ and on the right - at $\eta < 0$ (see Fig. 1.2).

If we search the relation between Cartesian and curvilinear coordinates in form of

$$x = \varphi_1(\xi) + a(\xi) \cdot \eta;$$
$$y = \varphi_2(\xi) + b(\xi) \cdot \eta,$$

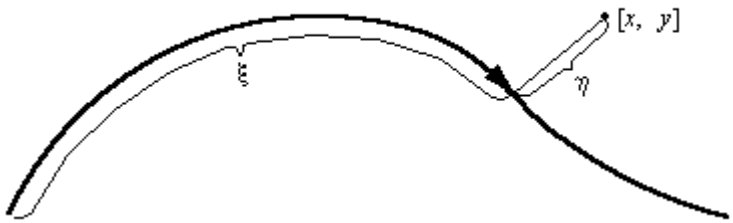


Figure 1.2. Curvilinear coordinates connected with the line.

then functions $a(\xi)$ and $b(\xi)$ can be determined from the condition of orthogonality of the curvilinear coordinate system taking into account that in this case nondiagonal components of the covariant metric tensor are equal to

$$g_{12} = (\dot{\varphi}_1(\xi) + \dot{a}(\xi) \cdot \eta) \cdot a(\xi) + (\dot{\varphi}_2(\xi) + \dot{b}(\xi) \cdot \eta) \cdot b(\xi) =$$
$$= \dot{\varphi}_1(\xi) \cdot a(\xi) + \dot{\varphi}_2(\xi) \cdot b(\xi) + \frac{\eta}{2} \cdot \frac{d}{d\xi}\left(\left(a(\xi)\right)^2 + \left(b(\xi)\right)^2\right).$$

The condition of orthogonality, apparently, will be executed if we suppose $a(\xi) = -\dot{\varphi}_2(\xi)$ and $b(\xi) = \dot{\varphi}_1(\xi)$.

The components of the covariant metric tensor of the coordinate system $\{\xi, \eta\}$ are equal to

$$g_{12} = g_{21} = 0; g_{22} = 1;$$
$$g_{11} = \left(\dot{\varphi}_1(\xi) - \ddot{\varphi}_2(\xi) \cdot \eta\right)^2 + \left(\dot{\varphi}_2(\xi) + \ddot{\varphi}_1(\xi) \cdot \eta\right)^2.$$

Practically sometimes it is required to determine $[\xi, \eta]$ the curvilinear coordinates of the point with given $[x, y]$ Cartesian coordinates. In particular, when inputting data for a computer program, which executes calculation of pollutants concentrations in fluvial water, it is more convenient for the user to operate with Cartesian coordinates of analyzers, the polluting objects and points of bank lines, while during implementation of the algorithm of

numerical solution of a diffusion equation it is more convenient to deal with curvilinear coordinates of these points and objects.

From (1.41) and (1.42), the set of equations follows:

$$\begin{aligned}&\left(x-\varphi_1(\xi)\right)\cdot\dot{\varphi}_1(x)+\left(y-\varphi_2(\xi)\right)\cdot\dot{\varphi}_2(\xi)=0;\\&-\left(x-\varphi_1(\xi)\right)\cdot\dot{\varphi}_2(\xi)+\left(y-\varphi_2(\xi)\right)\cdot\dot{\varphi}_1(\xi)=\eta.\end{aligned}$$

The parameter ξ is determined by solution of the first from these equations. The parameter η is determined from the second equation. If it is required to determine only module of parameter η (but not its sign), it is possible to use simpler expression which doesn't include derivatives

$$\eta^2=\left(x-\varphi_1(\xi)\right)^2+\left(y-\varphi_2(\xi)\right)^2.$$

1.4.2. Using Spline-Interpolation for Giving a Curve

The easiest way is to set a contour of the river and its bank lines by means of a sequence of points with given coordinates. The elementary way of approximation of the plane curve, given by means of the sequence of $(N+1)$ distinct points with Cartesian coordinates $[x_j, y_j]$ $(j=0,...,N)$, is its approximation by the polygonal line connecting the given points. Parametric equations of this polygon are as follows:

$$x=x_j+\frac{\Delta x_j}{\Delta s_j}(s-s_j);\quad y=y_j+\frac{\Delta y_j}{\Delta s_j}(s-s_j)\qquad \text{at } s_j\le s\le s_{j+1},$$

where s is natural parameter of the curve; $[s_j]_0^N$ is the sequence of values of this parameter determined by ratios

$$s_0=0;\quad \Delta s_j=\sqrt{\left(\Delta x_j\right)^2+\left(\Delta y_j\right)^2}.$$

Suppose, the curve is given in the form of a sequence of $(N+1)$ distinct nodes with Cartesian coordinates $[x_j, y_j]$ $(j=0,...,N)$. It is required to approximate this curve by a curve, which we shall call *interpolating spline-curve*, given in the parametric form

$$x=\varphi_1(\xi);\quad y=\varphi_2(\xi),$$

where ξ means natural parameter of this spline-curve. The following conditions similar to the conforming conditions for interpolating spline-functions [16] are superimposed on the functions $\varphi_1(\xi)$ and $\varphi_2(\xi)$, except for the requirement (1.41):

a) *condition of interpolating:* the interpolating curve passes through all given points, i.e. there is some sequence of values of a curve parameter $[\xi_j]_0^N$, for which the following takes place

$$\varphi_1(\xi_j) = x_j; \quad \varphi_2(\xi_j) = y_j \quad (j = 0,...,N)$$

(hereinafter the sequence $[\xi_j]$ everywhere is supposed increasing);

b) *smoothness of the curve:* the functions $\varphi_1(\xi)$ and $\varphi_2(\xi)$ are continuously differentiable on $[\xi_0, \xi_N]$;

c) *explicit form of functions:* in each of intervals $[\xi_j, \xi_{j+1}]$ $(j = 0,...,N-1)$ values of the functions $\varphi_1(\xi)$ and $\varphi_2(\xi)$, coincide with the corresponding values of the functions from the given class dependent on three additional parameters;

d) *boundary conditions:* the unit vector tangent to the curve has the given value in the point $[x_0, y_0]$.

1.4.3. Trigonometrical Spline-Interpolation

It is expedient to set the explicit form of functions $\varphi_1(\xi)$ and $\varphi_2(\xi)$, on each of the intervals $[\xi_j, \xi_{j+1}]$ so that the condition (1.41) will be executed automatically. One of the elementary types of these functions can be obtained from the condition that at $\xi_j \le \xi \le \xi_{j+1}$ the components of a unit vector τ tangent to the contour are equal to

$$\tau_x = -\sin(\zeta_j(\xi - \xi_j) + \varphi_j) = \cos(\zeta_j(\xi - \xi_j) + \varphi_j + 2\pi/4);$$
$$\tau_y = \cos(\zeta_j(\xi - \xi_j) + \varphi_j) = \sin(\zeta_j(\xi - \xi_j) + \varphi_j + 2\pi/4);$$

where ξ_j, ζ_j, φ_j $(j = 0,...,N)$ are constant coefficients.

Parametric equations of the curve in the interval $[\xi_j, \xi_{j+1}]$ are as follows: at $\zeta_j \neq 0$

$$x = \breve{x}_j + (1/\zeta_j) \cdot \cos(\zeta_j(\xi - \xi_j) + \varphi_j); \quad y = \breve{y}_j + (1/\zeta_j) \cdot \sin(\zeta_j(\xi - \xi_j) + \varphi_j);$$

at $\zeta_j = 0$

$$x = x_j - \sin\varphi_j \cdot (\xi - \xi_j) = x_j + \frac{\Delta x_j}{\Delta \xi_j}(\xi - \xi_j);$$

$$y = y_j + \cos\varphi_j \cdot (\xi - \xi_j) = y_j + \frac{\Delta y_j}{\Delta \xi_j}(\xi - \xi_j),$$

where $\breve{x}_j \ \ (j = 0,...,N)$ are additional constant coefficients, and the symbol Δ marks the ascending differences.

The values ξ_j, $\breve{x}_j$, ζ_j, φ_j are determined by the condition of smoothness of the curve in nodes and the boundary conditions for tangent vector to the curve in the point $[x_0, y_0]$. However, instead of equating values in the points ξ_j of the functions and their derivatives, given on intervals $[\xi_{j-1}, \xi_j]$ and $[\xi_j, \xi_{j+1}]$ and to derive thus equations for required parameters, we shall act as follows: we shall determine each of these parameters by means of the formulae of analytical geometry and elementary planimetry taking into account its geometrical sense (see Fig. 1.3).

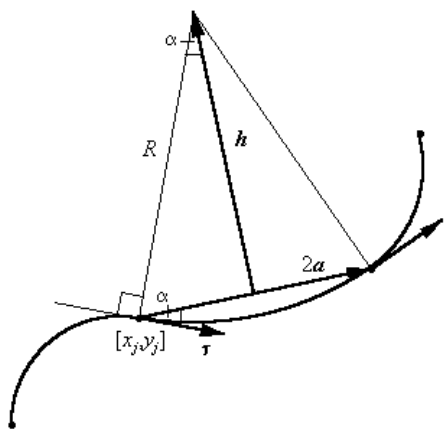


Figure 1.3. Trigonometrical Spline-Interpolation.

As a result for determination of values $\xi_j, \breve{x}_j, \zeta_j, \varphi_j$ we have the following scheme:

$$\xi_0 = 0; \ \ \varphi_0 = \arg(\tau_{0y} - i\tau_{0x}),$$

where τ_0 is the value of unit vector tangent to the curve in the point $[x_0, y_0]$; the remaining parameters sequentially are determined for all $j = 0,...,N-1$ by means of the following formulae:

$$\tau_y = \cos\varphi_j; \quad \tau_x = -\sin\varphi_j;$$

τ is unit vector tangent to the curve in the point $[x_j, y_j]$; $\varphi_j + 2\pi/4$ represents slope of this vector to a positive direction of the abscissa axis;

$$a_x = (x_{j+1} - x_j)/2; \quad a_y = (y_{j+1} - y_j)/2; \quad a = \sqrt{a_x^2 + a_y^2};$$

$2a$ is a position vector conducted from the point $[x_j, y_j]$ to the point $[x_{j+1}, y_{j+1}]$;

$$\cos\alpha = (\tau_x a_x + \tau_y a_y)/a; \quad \sin\alpha = (\tau_x a_y - \tau_y a_x)/a;$$

α is the angle, on which the vector τ should be turned to make it parallel to vector a;

$$\zeta_j = \sin\alpha / a;$$

$R = 1/|\zeta_j|$ is the radius of the arc of the circumference coincided with a part of the curve between its points $[x_j, y_j]$ and $[x_{j+1}, y_{j+1}]$; at $\zeta_j = 0$ this arc degenerates into a straight line segment; at $\zeta_j > 0$ the center of this arc $[\breve{x}_j, \breve{y}_j]$ is to the left of the curve, and at $\zeta_j < 0$ - on the right; therefore, at $\zeta_j > 0$ the arc is drawn from the point $[x_j, y_j]$ in $[x_{j+1}, y_{j+1}]$ counter-clockwise, and at $\zeta_j < 0$ - clockwise;

$$\varphi_{j+1} = \varphi_j + 2\alpha;$$

$$\xi_{j+1} = \begin{cases} \xi_j + 2\alpha/\zeta_j, & \text{at } \zeta_j \neq 0; \\ \xi_j + 2\alpha, & \text{at } \zeta_j = 0. \end{cases}$$

At $\zeta_j \neq 0$ there are determined also

$$h_x = -a_y / tg\alpha; \quad h_y = a_x / tg\alpha;$$

h is the position vector drawn from the bisecting point of the segment between points $[x_j, y_j]$ and $[x_{j+1}, y_{j+1}]$ into the center of the arc;

$$\breve{x}_j = (x_j + x_{j+1})/2 + h_x; \quad \breve{y}_j = (y_j + y_{j+1})/2 + h_y$$

are coordinates of the center of the arc.

The spline-curve, apparently, has no inflection points for values ξ belonging to internal points of each of intervals (ξ_j, ξ_{j+1}), i.e. nodes can be the only inflection points of the given curve.

1.4.4. Spline-Interpolation by Integrals of Fractional-Rational Functions

The offered below type of the functions specifying a spline-curve, is determined so that at $\xi_j \le \xi \le \xi_{j+1}$ the components of a unit vector τ tangent to the curve were be equal to

$$\tau_x = \frac{1-u^2}{1+u^2}; \quad \tau_y = \frac{2u}{1+u^2},$$

where

$$u = u_j + b_j(\xi - \xi_j),$$

ξ_j, u_j and $b_j (j = 0,..., N)$ are constants. The auxiliary function u represents tangent of half slope of tangent vector to the curve in the appropriate point to the positive direction of the abscissa axis.

The parametric equation of the curve in the interval $[\xi_j, \xi_{j+1}]$ is as follows: at $b_j \neq 0$

$$x = x_j - \xi + \xi_j + \frac{2}{b_j} \cdot arctg \frac{u - u_j}{1 + u_j u} =$$

$$= x_j - \xi + \xi_j + \frac{2}{b_j} \cdot arctg \frac{b_j(\xi - \xi_j)}{1 + u_j^2 + u_j b_j (\xi - \xi_j)};$$

$$y = y_j + \frac{1}{b_j} \cdot \ln \frac{1+u^2}{1+u_j^2} = y_j + \frac{1}{b_j} \cdot \ln \frac{1 + (u_j + b_j(\xi - \xi_j))^2}{1+u_j^2};$$

at $b_j = 0$

$$x = x_j + \frac{\Delta x_j}{\Delta \xi_j} \cdot (\xi - \xi_j); \quad y = y_j + \frac{\Delta y_j}{\Delta \xi_j} \cdot (\xi - \xi_j).$$

The values ξ_j, u_j and b_j are determined by the condition of smoothness of the curve in the nodes and boundary conditions for tangent vector to the curve in the point $[x_0, y_0]$. As a result for determination of these coefficients we have the following scheme:

$$\xi_0 = 0; \quad u_0 = \frac{\tau_{0y}}{1+\tau_{0x}} = \frac{1-\tau_{0x}}{\tau_{0y}},$$

where τ_0 is the value of a unit vector tangent to the curve in the point $[x_0, y_0]$; the remaining parameters are determined sequentially for all $j = 0,...,N-1$ by the formulae

$$b_j = \frac{\Delta u_j}{\Delta \xi_j} = \frac{1}{\Delta y_j} \ln \frac{1+u_{j+1}^2}{1+u_j^2} = \frac{1}{\Delta x_j}(u_j - u_{j+1} + 2arctg \frac{u_{j+1}-u_j}{1+u_j u_{j+1}}).$$

It is possible to show that the considered spline-curve, as well as in the previous example, has no inflection points for values ξ, belonging to internal points of each of intervals (ξ_j, ξ_{j+1}), i.e. nodes can be the only inflection points of the given curve.

For determination of each of parameters u_{j+1} it is necessary to solve a nonlinear equation. Therefore it is necessary correctly select the search interval of this parameter. If we write this equation in the following form $f(u) = 0$, the function $f(u)$ will have two extremums

$$\widetilde{u} = \frac{a_y / a}{1 + a_x / a} \quad \text{and} \quad \widetilde{u}' = \frac{-a_y / a}{1 - a_x / a},$$

where a is position vector conducted from the point $[x_j, y_j]$ to the point $[x_{j+1}, y_{j+1}]$. The parameters u_j, $\widetilde{u}$ and $\widetilde{u}'$ are determined by directions of vectors τ_j, a and $-a$, respectively: each of this parameters represents tangent of half slope of the appropriate vector to the positive direction of the abscissa axis; here τ_j is unit vector tangent to the curve in the point ξ_j. If the direction of tangent vector to the curve doesn't vary too hardly on the interval $[\xi_j, \xi_{j+1}]$, the desired value u_{j+1} is approximately equal to $\widetilde{u}$. At the same time the parameter $\widetilde{u}'$ corresponds to the opposite direction of the vector a and, therefore, there is no practical significance for determination of u_{j+1}.

Taking into account the absence of inflection points for the curve at $\xi_j < \xi < \xi_{j+1}$, as well as the execution of the equation $f(u) = 0$ at $u = u_j$ (that is clear from explicit form of the function $f(u)$), it is possible to show that $\widetilde{u}$ belongs to the interval with boundaries u_j and u_{j+1}. Geometrically it means that the vector a lies inside the angle formed by vectors τ_j and τ_{j+1} (see Fig. 1.3). Consequently, the desired value u_{j+1} belongs to the interval with boundaries $\widetilde{u}$ and $\widetilde{u} + c(\widetilde{u} - u_j)$, where c is some positive number.

1.4.5. Final Remarks

The approximation of the given contour by means of interpolating spline-curve from the reviewed above classes is good in such cases, when the number of available nodes of the contour is great enough, otherwise for large values of the parameter ξ the approximated curve can essentially differ from the given one. For example, if trigonometrical spline-interpolation is being used for approximating the sinusoid, given for equidistant values of abscissa with the interval 0.8, the interpolating curve, introduced in Fig. 1.4 will be obtained. In this figure the initial sinusoid is shown by the dotted line; the nodes are distinguished by their sizes. The similar picture is given by approximating this sinusoid using the interpolation by integrals of fractional rational functions.

If the number of known coordinates of the contour points is not great enough, it is possible to solve the above mentioned problem in the following way.

Let us represent the initial curve in the parametric form

$$x = \psi_1(t); \quad y = \psi_2(t),$$

where t is the length of the polygon line connecting the current point of the curve with all previous nodes. The functions $\psi_1(t)$ and $\psi_2(t)$ can be approximated by cubical splines [16]. In this case t does not serve as a natural parameter of the curve and, therefore, assignment of the approximating curve by means of cubical splines does not give the capability to work with curvilinear coordinates, introduced in the section 1.4.1. However such way of assignment of the approximating curve allows to compute approximate values of coordinates of initial curve in some additional points, thereby having increased number of available nodes, then approximating of an available contour by spline-curve by methods described in sections 1.4.3 and 1.4.4 is already possible.

For example, if we increase the number of nodes of the reviewed above sinusoid using above described method, inserting three additional nodes between each adjacent points, the approximating curve practically will merge with the given sinusoid.

The use of splines while approximating a plane curve has all advantages which are typical for splines used for approximating of ordinary numeric functions, namely: convergence, stability and relative simplicity of the mathematical expressions. In order to meet the requirement of the curve parameter's being natural, we had to refuse conventional ways of determination of splines by means polynomials.

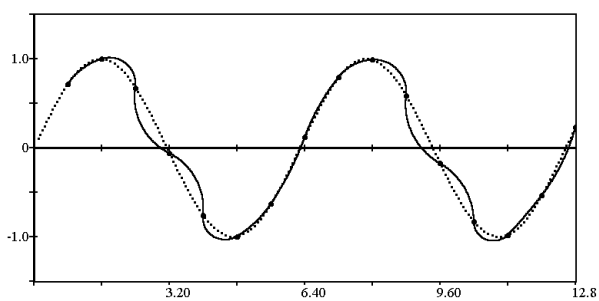


Figure. 1.4. Interpolating spline-curve for the sinusoid in case of infrequent nodes.

After we compare two offered methods of construction of splines: one - by means of trigonometrical functions and another - by means of integrals of fractional rational functions, it is possible to say, that advantage of the first method is the relative simplicity and reliability of calculations, its imperfection – more sensitivity to "rarefaction" of nodes.

The description of offered algorithms contains everything required for their implementation in form of computer programs. Such programs are drawn up by the authors of this work and are tested on many control examples and are used in computer packages "Application package of realization of mathematical models of pollutants transfer in rivers (MMPT)" (Version 2.0) [227] and "Automatic Detection of River Water Excessive Pollution Sources (ADrweps)" (Version 2.0) [210] described in Chapters 6 and 7.

1.5. ABOUT APPROXIMATION OF RIVER CURRENT SPEED

The problem of correct determination of river current speed is very important for the problem of modeling the transfer of pollutants in rivers. Despite this, in general case, it is not solved till now because of complexity and variety of variants depending on features of the rivers. We reduce one of practical ways of its solution below.

Geometrical characteristics of a channel of the river, on which the speed of a current depends, can strongly vary on a considered section, especially if the mountain river is investigated. From components of the vector of the current speed and their derivatives on spatial co-ordinates, in one's turn, coefficients of turbulent diffusion depend on. It is clear, that, generally, for speed of the current it is impossible to use simple linear interpolation in which values of the speed only on the section ends are considered, except any special cases when, for example, water flows on the rectangular channel. Practical obtaining values of the speed of the current in many points of the section, in general case, are very difficult and expensive problem. Therefore it is necessary to solve this problem analytically especially as the geometry of the section of the river unequivocally defines the speed of the current in any point of this section.

One of possible approaches to the solution of this problem consists in the following: to use linear interpolation for the dependence of the expense of water $P(r)$ on longitudinal co-ordinate, and by $P(r)$ to express values of the speed of the current $v(r) = P(r)/E(r)$, where $E(r)$ is the area of cross-section of the river in point r. Namely such method is realized in packages of applied programs described in Chapters 6 and 7. This method is simple, but, unfortunately, rough since it allows to determine only average value of the speed on all cross-section of the river.

For exact solution of this problem, apparently, it is impossible to go around solution of difficult equations of hydrodynamics – equations of Navier-Stokes or any simplified variant - of this equation, but necessarily considering viscosity of the water. The problem considerably will become simpler, if it succeeds to be reduced to the solution of some linear differential equation which can be solved, for example, by numerical methods.

Chapter 2

CALCULATION SCHEMATA OF MATHEMATICAL MODELS

2.1. NUMERICAL METHODS OF SOLVING DIFFUSION EQUATIONS

2.1.1. Boundary Problem

At solution of the diffusion equation, a boundary problem is considered as auxiliary [38, 40, 222, 223]. In this problem, unknown function $\Phi(x)$ is defined at $x \in X$, where X is the interval (in a one-dimensional problem) or the region (in a multivariable problem). The problem contains the differential equation

$$\hat{\alpha}\,\Phi(\boldsymbol{x}) = f(\boldsymbol{x})$$

and boundary conditions on the border of the region X

$$\hat{\beta}\,\Phi(\boldsymbol{x}) = \psi(\boldsymbol{x}),$$

where $f(x)$ and $\psi(x)$ are the given numerical functions; $\hat{\alpha}$ is the linear elliptic differential operator; $\hat{\beta}$ is the first-order linear differential operator.

At the solution of the boundary problem, the differential equation for internal points of the region X is replaced with the difference equation

$$\hat{\alpha}_h\,\Phi(\boldsymbol{x}) = f(\boldsymbol{x}),$$

where $\hat{\alpha}_h$ is the difference operator depending on additional parameter h, which is the maximum spatial step of the grid. The function $f_h(x)$ is equal to $f(x)$ - for internal points of the region X and some combination of the functions $\psi(x)$ and $f(x)$ for boundary points.

In the future, for the simplicity, in difference equations the index h is omitted so far as it does not complicate understanding of the essence of the presented material.

The accuracy of approximation of the differential operator $\hat{\alpha}$ by difference operator $\hat{\alpha}_h$ is characterized by misclosure $\rho(x,h)$:

$$\rho(\boldsymbol{x},h) = \hat{\alpha}_h\ \Phi(\boldsymbol{x}) - \hat{\alpha}\ \Phi(\boldsymbol{x}).$$

In the difference schemes considered below this approximation has the order h^2, i.e. at $h \to 0$

$$\rho(x,h) = O(h^2).$$

1. Review of difference schemes for one-dimensional boundary problem.

In the one-dimensional case, when $X = [a,b]$ is the interval, the operator $\hat{\alpha}$ is represented in the form of

$$\hat{\alpha} = -\frac{\partial}{\partial x}\left(A(x)\frac{\partial}{\partial x}\right) + B(x)\frac{\partial}{\partial x} + C(x) =$$
$$= -A(x)\frac{\partial^2}{\partial x^2} + \widetilde{B}(x)\frac{\partial}{\partial x} + C(x),$$

where $\widetilde{B}(x) = B(x) - \dot{A}(x)$; the boundary conditions are assigned in the form of

$$\left(p_a\ \Phi(x) + q_a\frac{\partial}{\partial \mathrm{x}}\Phi(x)\right)\Big|_{x=a} = \psi_a; \qquad \left(p_b\ \Phi(x) + q_b\frac{\partial}{\partial \mathrm{x}}\Phi(x)\right)\Big|_{x=b} = \psi_b.$$

Here $p_a, q_a, p_b, q_b, \psi_a, \psi_b = const$, $A(x), B(x), C(x)$ - the given numerical functions.

The difference operator $\hat{\alpha}_h$ is represented in the form of

$$\hat{\alpha}_h\ \Phi(\boldsymbol{x}) = \frac{1}{h^2}\left(G_{dn}(x,h)\cdot\Phi(x-h) + G_{md}(x,h)\cdot\Phi(x) + G_{up}(x,h)\cdot\Phi(x+h)\right),$$

where

$$G_{md}(x,h) = -G_{dn}(x,h) - G_{up}(x,h) + h^2\ C(x);$$

$$G_{up}(x,h) = -A(x) + \frac{h}{2}\widetilde{B}(x) + h^2\,U(x) + h^3\,V_{up}(x,h);$$

$$G_{dn}(x,h) = -A(x) - \frac{h}{2}\widetilde{B}(x) + h^2\,U(x) + h^3\,V_{up}(x,h);$$

$U(x)$, $V_{up}(x,h)$, $V_{dn}(x,h)$ are any four-time continuous-differentiable functions.

Different functions U, V_{up} and V_{dn} correspond to different difference schemes; in particular we may set:

$$G_{dn}(x,h) = -A(x-h/2) - \frac{h}{2}B(x); \qquad G_{up}(x,h) = -A(x+h/2) + \frac{h}{2}B(x) \tag{2.1}$$

The difference operator with such coefficients is used in practice most often.

Difference equation for the layers has the form: at $a < x < b$

$$\left(G_{dn}(x,h)\cdot\Phi(x-h) + G_{md}(x,h)\cdot\Phi(x) + G_{up}(x,h)\cdot\Phi(x+h)\right) = h^2 f(x);$$

at $x = a$

$$\left(G_{md}^{(a)}(h)\cdot\Phi(x) + G_{up}^{(a)}(h)\cdot\Phi(x+h)\right) = h^2 f^{(a)};$$

at $x = b$

$$\left(G_{dn}^{(b)}(h)\cdot\Phi(x-h) + G_{md}^{(b)}(h)\cdot\Phi(x)\right) = h^2 f^{(b)}.$$

Coefficients of this difference equation for the bounds of the interval $[a,b]$ are determined by the ratios: at $q_a = 0$

$$G_{up}^{(a)}(h) = 0; \qquad G_{md}^{(a)}(h) = p_a\,h; \qquad f^{(a)} = \psi_a; \tag{2.2}$$

at $q_a \neq 0$

$$G_{md}^{(a)}(h) = G_{md}(a,h) + \frac{2h\,p_a}{q_a}G_{dn}(a,h); \quad G_{up}^{(a)}(h) = G_{up}(a,h) + G_{dn}(a,h)$$

$$f^{(a)} = f(a) + \frac{2}{h\,q_a}G_{dn}(a,h)\cdot\psi_a; \tag{2.3}$$

at $q_b = 0$

$$G_{dn}^{(b)}(h) = 0; \quad G_{md}^{(b)}(h) = p_b\ h; \quad f^{(b)} = \psi_b, \tag{2.4}$$

at $q_b \neq 0$

$$G_{md}^{(b)}(h) = G_{md}(b,h) - \frac{2h\,p_b}{q_b} G_{up}(b,h); \quad G_{dn}^{(b)}(h) = G_{dn}(b,h) + G_{up}(b,h);$$

$$f^{(b)} = f(b) - \frac{2}{h\,q_b} G_{up}(b,h) \cdot \psi_b \,. \tag{2.5}$$

The given difference equations are equivalent to the system of $N+1$ linear equations for values of the function $\Phi(x)$ in equidistance nodal points $a + jh$ ($j = 0,...,N$), where $h = (b-a)/N$. The matrix of this system is three diagonal and, accordingly, the system of equations can be solved by the method of direct scrolling.

The substitution of the classical boundary conditions in the point b by non classical conditions is equivalent to the substitution of the latest equation in the given system by linear ratio between the values of the function $\Phi(x)$ in the point b and some internal point of the interval X. Such system of equations is solved by the special scrolling method [43].

2. Multidimensional boundary problem. Let us consider the *m*-dimensional boundary problem in the case when the region X is m-dimensional hyper parallelepiped, the coordinates of the points of which satisfy the inequalities:

$$a_k \le x_k \le b_k, \ (k = 1,...,m) \,.$$

The operator $\hat{\alpha}$ is represented in the form of

$$\hat{\alpha} = -\nabla \cdot (\mathbf{A}(\boldsymbol{x}) \cdot \nabla) + \boldsymbol{B}(\boldsymbol{x}) \cdot \nabla + C(\boldsymbol{x}) \,, \tag{2.6}$$

where $C(x)$, $B(x)$ and $A(x)$ are the second-rank scalar, vector and tensor depending on $\boldsymbol{x}$; the tensor $A(x)$ is considered as diagonal, which essentially simplifies the difference schemes.

The boundary conditions are set in the form of

$$\left(p_k^{(a)}\,\Phi(\boldsymbol{x})+q_k^{(a)}\,\nabla_k\Phi(\boldsymbol{x})\right)\Big|_{x_k=a_k}=\psi_k^{(a)}(x_1,...,x_{k-1},x_{k+1},...,x_m);$$
$$\left(p_k^{(b)}\,\Phi(\boldsymbol{x})+q_k^{(b)}\,\nabla_k\Phi(\boldsymbol{x})\right)\Big|_{x_k=b_k}=\psi_k^{(b)}(x_1,...,x_{k-1},x_{k+1},...,x_m),$$

$\left(k=1,...,m\right)$. Here $p_k^{(a)}$, $q_k^{(a)}$, $p_k^{(b)}$, $q_k^{(b)}=const$, $\psi_k^{(a)}$, $\psi_k^{(b)}$ are the given numerical functions.

The *m*-dimensional rectangular grid with equidistant nodes along the coordinate axes is used in the considered difference scheme. Thus the difference equation is equivalent to the set of N linear equations for the values of function $\Phi(\boldsymbol{x})$ at nodal points with coordinates $x_k=a_k+j_kh_k$ $\left(k=1,...,m;\,j_k=0,1,...,N_k\right)$, where $h_k=\left(b_k-a_k\right)/n_k$ are the spatial steps of the grid; $\left(n_k+1\right)$ is the number of nodal points along the k-th coordinate axis; $N=\left(n_1+1\right)\cdots\left(n_m+1\right)$ is the total number of nodal points which coincides with the order of the matrix corresponding to the difference operator $\hat{\alpha}_h$.

Diagonality of the tensor $A(x)$ means that $\hat{\alpha}$ is equal to the sum of m operators, each of which contains the derivatives only by one variable. The difference operator $\hat{\alpha}_h$, approximating $\hat{\alpha}$, also can be presented in the form of the sum of one-dimensional difference operators, the expressions for which can be derived from the corresponding formulae of the previous item.

2.1.2. Diffusion Equation

In the so-called mixed problem containing the diffusion equation, unknown function $\Phi\left(t,\boldsymbol{x}\right)$ is considered defined at $t\geq 0$ and $\boldsymbol{x}\in X$, where X is the interval (in the one-dimensional problem) or the region (in the multivariable problem). The problem contains differential equation

$$D(t,\boldsymbol{x})\frac{\partial}{\partial t}\Phi(t,\boldsymbol{x})+\hat{\alpha}(t)\,\Phi(t,\boldsymbol{x})=f(t,\boldsymbol{x}), \tag{4}$$

zero condition $\Phi\left(0,\boldsymbol{x}\right)=\Phi_0\left(\boldsymbol{x}\right)$ and boundary conditions on the border of the region X

$$\hat{\beta}(t)\,\Phi(t,\boldsymbol{x})=\psi(t,\boldsymbol{x}),$$

where $D(t,\boldsymbol{x})$, $f(t,\boldsymbol{x})$, $\psi(t,\boldsymbol{x})$ and $\Phi_0(\boldsymbol{x})$ are the given numerical functions; $\hat{\alpha}(t)$ is the linear elliptic differential operator depending on t; $\hat{\beta}(t)$ is the first-order linear differential operator depending on t.

1. Review of classical difference methods. At the use of the classical algorithm, rather small step of digitization of time τ is chosen, and the considered diffusion equation is

replaced with the following difference equation:

$$\frac{1}{\tau} D(t+\nu\tau, \boldsymbol{x}) \cdot \left(\widetilde{\Phi}(t+\tau, \boldsymbol{x}) - \widetilde{\Phi}(t, \boldsymbol{x})\right) + \\ + \sigma \cdot \hat{\alpha}(t+\nu\tau)\, \widetilde{\Phi}(t+\tau, \boldsymbol{x}) + (1-\sigma) \cdot \hat{\alpha}(t+\nu\tau)\, \widetilde{\Phi}(t, \boldsymbol{x}) = \\ = f(t+\nu\tau, \boldsymbol{x}), \tag{2.7}$$

where σ and ν are any real parameters; $0 \le \nu \le 1$; $\widetilde{\Phi}$ is grid function.

Different values of the given parameters correspond to different schemes; in particular we may put:

a) $\sigma = 0$; $\nu = 0$ (*the explicit scheme*);
b) $\sigma = 1$; $\nu = 0$ (*the cleanly implicit scheme*);
c) $\sigma = 1/2$; $\nu = 1/2$ (*the symmetric scheme*).

The symmetric scheme provides the accuracy of order τ^2; for all other schemes the accuracy of order τ is reached. At $\sigma \ge 1/2$, the stability of the scheme is guaranteed at any τ and h values (see [16]).

If exact or approximate values of function $\Phi(t, \boldsymbol{x})$ are known for some value t the problem of determination of the values of this function at the moment $t+\tau$ is reduced to solution of the boundary problem. Let us designate (for given value t):

$$\Phi_{lau}(\boldsymbol{x}) = \Phi(t+\tau, \boldsymbol{x}); \qquad \Phi_{last}(\boldsymbol{x}) = \Phi(t, \boldsymbol{x}); \\ t' = t + \nu\tau; \\ \hat{\alpha}_{lau} = \sigma \cdot \hat{\alpha}(t') + \frac{1}{\tau} D(t', \boldsymbol{x}) \cdot \hat{I}; \\ f_{lau}(\boldsymbol{x}) = f(t', \boldsymbol{x}) + \frac{1}{\tau} D(t', \boldsymbol{x}) \cdot \Phi_{last}(\boldsymbol{x}) - (1-\sigma) \cdot \hat{\alpha}(t')\, \Phi_{last}(\boldsymbol{x}); \\ \hat{\beta}_{lau} = \hat{\beta}(t+\tau); \qquad \psi_{lau} = \psi(t+\tau, \boldsymbol{x}). \tag{2.8}$$

The function $\Phi_{lau}(\boldsymbol{x})$ satisfies the so-called equation for layers

$$\hat{\alpha}_{lau}\, \Phi_{lau}(\boldsymbol{x}) = f_{lau}(\boldsymbol{x}), \tag{2.9}$$

(this is an approximate equation which represents other form of writing equation (2.7)) and the boundary conditions

$$\hat{\beta}_{lau}\, \Phi_{lau}(\boldsymbol{x}) = \psi_{lau}(\boldsymbol{x}).$$

Thus, equation (2.7) allows us to determine in succession the values of function $\Phi(t, \boldsymbol{x})$ for $t = k\tau \ \ (k = 1,2,...)$.

2. Reduction of the multi-dimensional diffusion equation to the one-dimensional. Described below algorithm of solution of diffusion equation is used in multi-dimensional problems and is an alternative to the considered above algorithms. In this algorithm solution of the multi-dimensional diffusion equation is presented as linear combination of solutions of some one-dimensional diffusion equations [30, 43]. This method is often called the method of splitting of operator or the method of decomposition of the multi-dimensional operator.

Analogously of the above considered algorithm, the region X transforms into the hyper parallelepiped and is accepted that after such transformation the operator $\hat{\alpha}(t)$, appearing in diffusion equation, is equal to the sum of m operators $\hat{\alpha}^{(k)}(t)$ each of which contains the derivatives only by one spatial co-ordinate. If for some value of t the exact or approximate values of the function $\Phi_{last}(x) = \widetilde{\Phi}(t, \boldsymbol{x})$ are known, then the function $\widetilde{\Phi}(t, \boldsymbol{x})$ for next layer is presented in the form

$$\widetilde{\Phi}(t+\tau, \boldsymbol{x}) \approx \frac{1}{m}\sum_{k=1}^{m} \Phi^{(k)}(\boldsymbol{x}),$$

where each of functions $\Phi^{(k)}(\boldsymbol{x})$ is the solution of one-dimensional boundary problem

$$\hat{\alpha}_{lau}^{(k)}\ \Phi^{(k)}(\boldsymbol{x}) = f_{lau}^{(k)}(\boldsymbol{x});$$
$$\hat{\beta}_{lau}^{(k)}\ \Phi^{(k)}(\boldsymbol{x}) = \psi_{lau}(\boldsymbol{x}) \ \text{ at } x_k = a_k \ \text{ or } \ x_k = b_k\ ;$$

the value appearing in these equations are determined by the ratios, analogous of (2.8):

$$\hat{\alpha}_{lau}^{(k)} = \frac{1}{2}\hat{\alpha}^{(k)}(t+\tau/2) + \frac{1}{m\tau} D(t+\tau/2, \boldsymbol{x});$$
$$f_{lau}^{(k)}(\boldsymbol{x}) = \frac{1}{m} f(t+\tau/2, \boldsymbol{x}) + \frac{1}{m\tau} D(t+\tau/2, \boldsymbol{x}) \cdot \Phi_{last}(\boldsymbol{x}) - \frac{1}{2}\hat{\alpha}^{(k)}(t+\tau/2)\,\Phi_{last}(\boldsymbol{x});$$
$$\hat{\beta}_{lau} = \hat{\beta}(t+\tau); \quad \psi_{lau}(\boldsymbol{x}) = \psi(t+\tau, \boldsymbol{x}).$$

This scheme is steady and provides the accuracy $O(\tau + h^2)$ at approximation of the operator $\hat{\beta}_{lau}$ by ratios (2.2) – (2.5).

2.2. FINITE-DIFFERENCE AND ANALYTICAL METHODS OF SOLUTION OF ONE-DIMENSIONAL IN SPACE MODELS OF POLLUTANTS TRANSFER

Finite-difference approximation

Below are given difference schemes for models (1.31) and (1.32), at classical and non classical zero and boundary conditions.

Grid: $\varpi_{th} = \varpi_\tau \times \varpi_h,$

$$\varpi_\tau = \{t = t_n, t_n = n\tau, n = 0,1,..., N_t\}, \quad N_t = \left[\frac{T_{\max}}{\tau}\right];$$

$$\varpi_h = \{x_i, x_0 = a, x_N = b, i = 0,1,..., N\};$$

$$x_i = x_{i-1} + h_i, \quad h_i > 0, \quad h_i^* = (h_i + h_{i+1})/2, \quad i = 1,..., N-1;$$

$$x_{N-K_\xi} = \xi.$$

K_ξ is a natural number denoting the number of nodes from the inner cross-section to the end of the controlled section.

The finite-difference analog of the equation is:

$$E_j \cdot \frac{Y_j^{n+1} - Y_j^n}{\tau} = \Lambda\left(\sigma Y_j^{n+1} + \overline{\sigma} Y_j^n\right) + \sigma f_j^{n+1} + \overline{\sigma} f_j^n, \tag{2.10}$$

where $0 \le \sigma \le 1, \quad j = 1,..., N-1, \quad n = 0,1,..., N_t - 1,$

$$\Lambda Y_j = \left(a Y_{\bar{x}}\right)_{\hat{x},j} - \frac{1}{2}\left((bY)_{x,j} + (bY)_{\hat{x},j}\right) - K_j Y_j,$$

$$a_j = E\left(x_{j-1/2}\right) \cdot K\left(x_{j-1/2}\right), \quad b_j = E\left(x_j\right) \cdot v(x_j), \quad \zeta_j = \zeta\left(x_j\right), \quad E_j = E\left(x_j\right).$$

Approximation of the initial data:

$$Y_j^0 = \Phi_{10}\left(x_j\right), \quad j = 0,1,..., N, \tag{2.11}$$

Approximation of the boundary condition at the entrance of the section:

$$Y_0^n = \Phi_a(t_n), \quad n = 0,1,..., N_t, \tag{2.12}$$

The finite-difference analog at the boundary condition of full mixing:

$$\tau\sigma K(x_N)(Y_N - Y_{N-1}) + \tau\overline{\sigma}(\hat{Y}_N - \hat{Y}_{N-1}) + \hat{Y}_N - Y_N + (vE)'_{xN}(\sigma\hat{Y}_N + \overline{\sigma}Y_N) = 0. \tag{2.13}$$

Approximation of the nonlocal condition;

$$Y_N^n = qY_{N-K(\xi)}^n + \omega^n. \tag{2.14}$$

The following notation was used above:

$$Y_x = (Y_{j+1} - Y_j)/h_j, \quad Y_{\bar{x}} = (Y_j - Y_{j-1})/h_{j-1}, \quad Y_{\hat{x}} = \frac{Y_{j+1} - Y_j}{h_j^*}. \tag{2.15}$$

The difference scheme for model (1.31), (1.32), (1.37) is described by formulae (2.10), (2.11), (2.12), (2.13), and for model (1.31), (1.32), (1.38) - by formulae (2.10), (2.11), (2.12), (2.14).

2.3. ALGORITHMIC PRESENTATION OF THE FINITE-DIFFERENCE METHOD

Realization of the finite-difference scheme is reduced to the solution of the following system of linear algebraic equations:

$$A_i Y_{i-1} - C_i Y_i + B_i Y_{i+1} = -S_i, \quad i = 1,2,..., N-1, \tag{2.16}$$

$$Y_0 = E_0, \tag{2.17}$$

$$Y_N = qY_{N-K(\xi)} + E_N. \tag{2.18}$$

where

$$A_i = \sigma\tau\left(\frac{D_{i+1}}{h_i^* h_{i+1}} - \frac{1}{2}\nu_{i+1}EE_{i+1}\right)/EE_i, \tag{2.19}$$

$$C_i = 1 + \sigma\tau\left(\left(\frac{D_{i+1}}{h_i^* h_{i+1}} + \frac{D_i}{h_i^* h_i}\right) - \frac{1}{2}\left(\frac{\nu_i}{h_{i+1}} - \frac{\nu_i}{h_i}\right)EE_i + K_i\right)/EE_i, \tag{2.20}$$

$$B_i = \sigma\tau\left(\frac{D_i}{h_i^* h_i} - \frac{1}{2}\frac{\nu_{i-1}EE_{i-1}}{h_i}\right)/EE_i, \tag{2.21}$$

$$S_i = -\tau E_i / EE_i - \left(\Phi_i + \tau(1-\sigma)\left(\frac{D_i}{h_i^* h_{i+1}}(\Phi_{i+1} - \Phi_i) - \frac{D_i}{h_i^* h_i}(\Phi_i - \Phi_{i-1}) - \right.\right.$$
$$\left.\left. - \frac{EE_{i+1}\nu_{i+1}\Phi_{i+1} - EE_i \nu_i \Phi_i}{2h_{i+1}} - \frac{\nu_i \Phi_i - \nu_{i-1}\Phi_{i-1}}{2h_i} \right) / EE_i - \tau\bar{\sigma} K_i \Phi_i / EE_i \right), \tag{2.22}$$

$$D_i = K(x_i) \cdot EE_i, \tag{2.23}$$

$q = q(S)$ and $\Phi_N = \Psi$ in case of non-local boundary condition,

$$S_N = \left(\tau\sigma D_N \Phi_{N-1} + \left(1 - \sigma D_N (1 + EE_N \nu_N - EE_{N-1}\nu_{N-1})\Phi_N\right)\right) / \tilde{q},$$
$$\tilde{q} = 1 + \tau\bar{\sigma} D_N (1 + EE_N \nu_N - EE_{N-1}\nu_{N-1}),$$
$$q = 1 + \tau\bar{\sigma} D_N / \tilde{q}, \tag{2.24}$$

in case of the condition of full mixing.

For solving the system of linear algebraic equations (2.17)-(2.24) the method of scrolling is used in case of boundary condition of full mixing, and the modified run method - in case of non-local boundary condition. The algorithm is given below:

a) Calculation of scrolling coefficients:

$$\alpha_{i+1} = B_i / (C_i - \alpha_i A_i); \quad \beta_{i+1} = (A_i \beta_i + S_i)/(C_i - \alpha_i A_i); \quad i = 1,2,...,N-1;$$
$$\alpha_1 = 0, \quad \beta_1 = S_0.$$

b) Calculation of Y_N :

$$Y_N = (q\beta_N + S_N)/(1 - q\alpha_N), \text{ when } K(\xi) = 1,$$
$$Y_N = \frac{\sum_{l=0}^{K(\xi)-1} \left(\prod_{K=l+1}^{K(\xi)-1} \alpha_{N-k} \right) \beta_{N-l} + S_N}{1 - q \prod_{k=0}^{K(\xi)-1} \alpha_{N-k}}, \text{ when } K(\xi) > 1,$$

c) Calculation of solution:

$$Y_i = \alpha_{i+1} Y_{i+1} + \beta_{i+1}, \quad i = N-1, N-2,...,1.$$

In addition, were considered one-dimensional problems of river water pollutants transfer and diffusion on straight line $-\infty < x < +\infty$ and half-line $x \geq 0$, on the assumption that the river flow velocity and coefficients of turbulent diffusion are constant, and the pollutants are

non-conservative, in conditions when the water object is under the action of R independent pollution sources located at $x = x_r$ points of the section under consideration. Their solutions are represented in terms of one-dimensional integrals of the functions, which describe distributions of pollution sources and initial concentrations of pollutants, as well as (in case of half-line $x \geq 0$) pollution modes at boundary $x = 0$ [1]. These solutions are supposed to be used in investigations of qualitative peculiarities of pollutants transfer and of efficiency and accuracy of calculation methods on the base of one-dimensional as well as two- and three-dimensional models.

Separately were considered pollution problems: on the half-line with a stationary point-source and in stationary pollution mode at boundary $x = 0$. Solution of the latter, in the absence of initial pollutions, is reduced to the known error probability integral and is calculated particularly simply.

2.4. ALGORITHMS FOR SOLVING TWO-DIMENSIONAL MATHEMATICAL MODELS

For approximate solution of the problem (1.33), (1.34), the suitable numerical methods were developed on the basis of finite-difference method. In particular, for numerical solution of the stated problems there were developed the explicit scheme, the method of splitting the operator and the method of approximate factorization. Each of these methods has its advantages and lacks which the most fully appear on the stage of algorithmization.

Let us consider that the water course occupies region G in space of points $M \equiv (x, y, z)$; x, y, z are coordinates of point M in the orthogonal system of coordinates; axis x is directed along the averaged water flow velocity, y is directed from the surface level of water course downward, z is directed transverse to water course, orthogonally to plane (xOy).

The most general two-dimensional equation with the initial and boundary conditions is given in the previous paragraph. If pollutant concentration along transverse axis z is assumed to be unchangeable, then, in equation (1.33), it must be stated that $x_1 \equiv x$, $x_2 \equiv y$; if pollutant concentration remains unchangeable along y, then, in (1.33) it must be stated that $x_1 \equiv x$, $x_2 \equiv z$,; allowing for the above-stated, the boundary and initial conditions will assume the corresponding forms.

Let us assume that $G = \{(x_1, x_2),\ x_1 \in (0, \ell_1),\ x_2 \in (0, \ell_2)\}$ where ℓ_1 - is the averaged length of water course, ℓ_2 - either averaged width or depth. In this case we'll have:

$$\Gamma_1 = \{(x_1, x_2),\ x_1 = 0,\ 0 < x_2 < \ell_2\},$$

$$\Gamma_2 = \{(x_1, x_2),\ x_2 = \ell_2,\ 0 < x_1 < \ell_1\},$$

$$\Gamma_3 = \{(x_1, x_2),\ x_1 = \ell_1,\ 0 < x_2 < \ell_2\},$$

$$\Gamma_4 = \{(x_1, x_2),\ x_2 = 0,\ 0 < x_1 < \ell_1\},$$

$$\Gamma_0 = \{(x_1, x_2),\ x_1 = \xi,\ 0 < \xi < \ell_1,\ 0 < x_2 < \ell_2\}\}.$$

Taking into account above mentioned, the zero and boundary conditions for equation (1.33), (1.34) have the suitable form:

$$\Phi_i(0, x_1, x_2) = \Phi_{i0}(x_1, x_2),\ (x_1, x_2) \in G, \tag{2.25}$$

$$\Phi_i(t, x_1, x_2) = \varphi_i(t, x_1, x_2),\ (x_1, x_2) \in \Gamma_1,\ t > 0, \tag{2.26}$$

$$K_{1i}\frac{\partial \Phi_i}{\partial x_1}n_1 + K_{2i}\frac{\partial \Phi_i}{\partial x_2}n_2 + x_i\Phi_i = \psi_i,\ (x_1, x_2) \in \Gamma_2 \bigcup \Gamma_4,\ t > 0, \tag{2.27}$$

$$\frac{\partial \Phi_i}{\partial n} = 0,\ (x_1, x_2) \in \Gamma_3 \text{ (classical statement)}, \tag{2.28}$$

or

$$\Phi_i(t, x_1, x_2) = q\Phi_i(t, x_{10}, x_{20}) + \omega_i(t, x_1, x_2) \text{ (non-local statement)}, \tag{2.29}$$

$$(x_1, x_2) \in \Gamma_3,\ (x_{10}, x_{20}) \in \Gamma_0,$$

$$\Gamma_0 = \left\{(x_{10}, x_{20}) : (x_{10}, x_{20}) = I(x),\ x \in \Gamma_3\right\},$$

where I is diffeomorfizm, Γ_0 is the curve in G having unique points of intersection with Γ_2 and Γ_4, and these points do not coincide with the points of intersection of Γ_i, $i = 1,2,3,4.$

$\Phi_{i0}, \varphi_i, \psi_i, \omega_i$ are given functions, $q = const,\ 0 < q < 1;\ n = (n_1, n_2)$ is external normal.

The algorithm for solving problem (1.33), (1.34), (2.25)-(2.28) or (1.33), (1.34), (2.25)-(2.27), (2.29) is based on the method of operator decomposition. Time grid

$$\omega_\tau = \left\{t,\ t = t_j = j\tau,\ \tau = \frac{T}{K},\ j = 0,1,...,K\right\}.$$

is introduced. The split problem of decomposition method for (1.33), (1.34), (2.25)-(2.28) or (1.33), (1.34), (2.25)-(2.27), (2.29) may be stated in the following way: to find the solution of equations

$$0{,}5(\overline{\Phi}_i^{(j+1)})_t' = \frac{\partial}{\partial x_1}\left[k_{1i}\frac{\partial \overline{\Phi}_i^{(j+1)}}{\partial x_1}\right] - \frac{\partial}{\partial x_1}\left[\nu_1 \overline{\Phi}_i^{(j+1)}\right] - 0{,}5k\overline{\Phi}_i^{(j+1)} + f_1(t,x_1,x_2),$$

$$0{,}5(\overline{\overline{\Phi}}_i^{(j+1)})_t' = \frac{\partial}{\partial x_2}\left[k_{2i}\frac{\partial \overline{\overline{\Phi}}_i^{(j+1)}}{\partial x_2}\right] - \frac{\partial}{\partial x_2}\left[\nu_2 \overline{\overline{\Phi}}_i^{(j+1)}\right] - 0{,}5k\overline{\overline{\Phi}}_i^{(j+1)} + f_2(t,x_1,x_2), \qquad (2.30)$$

$$t_j < t \le t_{j+1}, \quad 0 < x_j < l_\alpha, \quad (\alpha = 1{,}2),$$

which satisfies initial conditions

$$\overline{\Phi}_i^{(j+1)}(t_j,x_1,x_2) = \widetilde{\Phi}_i^{(j+1)}(t_j,x_1,x_2),$$

$$\overline{\overline{\Phi}}_i^{(j+1)}(t_j,x_1,x_2) = \widetilde{\Phi}_i^{(j+1)}(t_j,x_1,x_2),$$

$$\widetilde{\Phi}_i^{(j+1)}(t_j,x_1,x_2) = 0{,}5\left[\overline{\Phi}_i^{(j+1)}(t_j,x_1,x_2) + \overline{\overline{\Phi}}_i^{(j+1)}(t_j,x_1,x_2)\right], \qquad (2.31)$$

$$\overline{\Phi}_i^{(0)}(0,x_1,x_2) = \overline{\overline{\Phi}}_i^{(0)}(0,x_1,x_2) = \Phi_0(x_1,x_2);$$

and boundary conditions

$$\overline{\Phi}^{(j+1)}(t,0,x_2) = \varphi_{1i}(t,x_1), \ 0 \le x_2 \le l_2, \ t_j \le t \le t_{j+1}, \qquad (2.32)$$

$$\overline{\Phi}_i^{(j+1)}(t,l_1,x_2) = q\overline{\Phi}_i^{(j+1)}(t,\xi,x_2), \ 0 \le x_2 \le l_2, \ t_j \le t \le t_{j+1}, \qquad (2.33)$$

$$k_{1i}\frac{\partial \overline{\overline{\Phi}}_i^{(j+1)}}{\partial x_2} + \chi_{1i}\overline{\overline{\Phi}}_i^{(j+1)} = \psi_{1i}, \ 0 \le x_1 \le l_1, \ x_2 = 0,$$

$$k_{2i}\frac{\partial \overline{\overline{\Phi}}_i^{(j+1)}}{\partial x_2} - \chi_{2i}\overline{\overline{\Phi}}_i^{(j+1)} = \psi_{2i}, \ 0 \le x_1 \le l_1, \ x_2 = l_2, \qquad (2.34)$$

$$t_j \le t \le t_{j+1}, \ j = 0,1,...,K-1,$$

where $f_{1i} + f_{2i} = E_i$, $\chi_{1i} \ge \chi_{01i} = const > 0$, $\chi_{2i} \ge \chi_{02i} = const > 0$.

We'll consider $\widetilde{S}_i^{(j+1)}(t,x_1,x_2)$ to be the solution of problem (2.30)-(2.34). It is proved [214-217], that $\widetilde{\Phi}_i^{(j+1)}(t,x_1,x_2)$ is the approximate solution of initial two-dimensional problem (1.33), (1.34), (2.25)-(2.27), (2.29).

Thus, the scheme of splitting (2.30)-(2.34) approximates non-classical-non-local problem (1.33), (1.34), (2.25)-(2.27), (2.29).

If condition (2.33) is changed by condition

$$\frac{\partial \overline{\Phi}_i^{(j+1)}}{\partial x_1} = 0 \text{ at } x_1 = \ell_1,\ 0 \le x_2 \le \ell_2,\ t_j \le t \le t_{j+1}, \tag{2.35}$$

then the problem (2.30)-(2.32), (2.34), (2.35) will approximate classical problem (1.33), (1.34), (2.25)-(2.28). Theoretical substantiation of such splitting exists [216].

Problems (2.30)-(2.34) and (2.30)-(2.32), (2.34), (2.35) may be solved by different methods. We have constructed effective finite-difference schemes for their solution [217, 218].

In case of classical boundary conditions, the method of scrolling is used for solving the received tree-point equations [219]. In case of non-classical boundary conditions, the scrolling formulae of special type are derived [30, 221].

2.5. ALGORITHMS FOR REALIZATION OF THREE-DIMENSIONAL DIFFUSION MODELS

Transport equation for the i_1th pollutant discharged by the i_2 th pollution source, in natural coordinate system, for a prismoidal river-bed with a rectangular cross-section, has the following form:

$$\frac{\partial \Phi_{i_1,i_2}}{\partial t} = \frac{\partial}{\partial x}.(K_{i_1,x}.\frac{\partial \Phi_{i_1,i_2}}{\partial x}) + \frac{\partial}{\partial y}.(K_{i_1,y}.\frac{\partial \Phi_{i_1,i_2}}{\partial y}) +$$
$$+ \frac{\partial}{\partial z}.(K_{i_1,z}.\frac{\partial \Phi_{i_1,i_2}}{\partial z}) - V\frac{\partial \Phi_{i_1,i_2}}{\partial x} - \zeta.\Phi_{i_1,i_2} + f_{i_1,i_2}, \tag{2.36}$$
$$0 < x < \ell_1,\ -\ell_2 < y < \ell_2,\quad 0 < z < \ell_3,\quad 0 < t < T,$$

where $K_{i_1,x} \equiv K_{i_1,x}(x,y,z,t)$, $K_{i_1,y} \equiv K_{i_1,y}(x,y,z,t)$, $K_{i_1,z} \equiv K_{i_1,z}(x,y,z,t)$, $V \equiv v(x,y,z,t)$, $K \equiv k(x,y,z,t)$, $f_{i_1,i_2} \equiv f_{i_1,i_2}(x,y,z,t)$ are known functions; x is a coordinate along the averaged watercourse velocity; y is a transverse coordinate; z is a coordinate along the watercourse depth; $S_{i_1,i_2} \equiv S_{i_1,i_2}(x,y,z,t)$ is the concentration of the i_1 th pollutant discharged from the i_2 th pollution source - the function to be found.

For equation (2.42), initial and boundary conditions must be specified:
initial condition

$$\Phi_{i_1,i_2}(x,y,z,0) = \Phi^0{}_{i_1,i_2}(x,y,z)$$

$$0 \le x \le \ell_1,\ -\ell_2 \le y \le \ell_2,\ 0 \le z \le \ell_3; \tag{2.37}$$

boundary conditions

$$\Phi_{i_1,i_2}(0,y,z,t) = \Phi_{0\ i_1,i_2}(y,z,t), \tag{2.38}$$

$$0 \le z \le \ell_3,\ -\ell_2 \le y \le \ell_2,\ 0 \le t \le T\ ;$$

$$\frac{\partial \Phi_{i_1,i_2}(x,y,z,t)}{\partial z}\Big|_{x=\ell_1} = 0,\ 0 \le z \le \ell_2,\ -\ell_2 \le y \le \ell_2,\ 0 \le t \le T\ ; \tag{2.39}$$

$$\frac{\partial \Phi_{i_1,i_2}(x,y,z,t)}{\partial y}\Big|_{x=-\ell_2} = \frac{\partial \Phi_{i_1,i_2}(x,y,z,t)}{\partial y}\Big|_{x=\ell_2} = 0, \tag{2.40}$$

$$0 \le x \le \ell_1,\ 0 \le z \le \ell_3,\ 0 \le t \le T;$$

$$\frac{\partial \Phi_{i_1,i_2}(x,y,z,t)}{\partial z}\Big|_{z=0} = \frac{\partial \Phi_{i_1,i_2}(x,y,z,t)}{\partial z}\Big|_{z=\ell_3} = 0, \tag{2.41}$$

$$0 \le x \le \ell_1,\ -\ell_2 \le y \le \ell_2,\ 0 \le t \le T.$$

Here $\Phi^0{}_{i_1,i_2}$ and $\Phi_{0\ i_1 i_2}$ are prescribed functions.

Instead of condition (2.39), the following non-local condition may be taken:

$$\Phi_{i_1,i_2}(\ell_1,y,z,t) = q\Phi_{i_1,i_2}(\xi,y,z,t), \tag{2.42}$$
$$-\ell_2 \le y \le \ell_2,\ 0 \le z \le \ell_3,\ 0 \le t \le T,$$

where q is a coefficient of self-purification and $0 \le q \le 1$.

Thus, we have two models: model (2.36)-(2.41) and model (2.36)-(2.38), (2.40), (2.41), (2.42) with non-local condition.

Let us consider space and time grids:

$$\omega_x = \left\{ x_i = ih_1,\quad i = 0,1,...,N_1,\quad h_1 = \frac{\ell_1}{N_1} \right\},$$

$$\omega_y = \left\{ Y_k = -\ell_2 + \mathrm{kh}_2,\quad k = 0,1,...,2N_2,\quad h_2 = \frac{\ell_2}{N_2} \right\},$$

$$\omega_z = \left\{ Z_m = mh_3,\quad m = 0,1,...,N_3,\quad h_3 = \frac{\ell_3}{N_3} \right\},$$

$$\omega_t = \left\{ t_j = j\tau,\quad j = 0,1,...,K,\quad K = \left[\frac{T}{\tau}\right] \right\},$$

where h_1, h_2, h_3 are grid spacings; τ is grid time interval; N_1, N_2, N_3, K are natural numbers.

For construction of a difference scheme, the method of decomposition of a multidimensional operator into one-dimensional ones is used.

The efficient algorithm given below is a difference scheme of parallel calculation with averaging.

Henceforth, values of some function, e.g. $\Phi(x, y, z, t)$, in grid nodes will be denoted in the following way:

$$\Phi(x_i, y_k, z_m, t_j) \equiv \Phi(i, k, m, j).$$

The scheme of parallel calculation with averaging is of the following form:

$$\frac{1}{3}\frac{\overset{(l)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\dot{\Phi}_{i_1,i_2}(i,k,m,j)}{\tau}=\frac{1}{h_1}\left\{k_{i_1,x}\left(i+\frac{1}{2},k,m,j+\frac{1}{2}\right)\times\frac{\overset{(l)}{\Phi}_{i_1,i_2}(i+1,k,m,j+1)-\overset{(l)}{\Phi}_{i_1,i_2}(i,k,m,j+1)}{h_1}-\right.$$

$$\left.-k_{i_1,x}\left(i-\frac{1}{2},k,m,j+\frac{1}{2}\right)\times\frac{\overset{(l)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\overset{(l)}{\Phi}_{i_1,i_2}(i-1,k,m,j+1)}{h_1}\right\}-V\left(i,k,m,j+\frac{1}{2}\right)\times$$

$$\times\frac{\overset{(l)}{\Phi}_{i_1,i_2}(i+1,k,m,j+1)-\overset{(l)}{\Phi}_{i_1,i_2}(i-1,k,m,j+1)}{2h_1}-\zeta\left(i,k,m,j+\frac{1}{2}\right)\overset{(l)}{\Phi}_{i_1,i_2}(i+1,k,m,j+1)+\frac{1}{3}f_{i_1,i_2}\left(i,k,m,j+\frac{1}{2}\right), \tag{2.43}$$

$(i=1,\ldots,N_1-1),\ \forall k,m,$

$$\dot{\Phi}_{i_1,i_2}(i,k,m,j)=\frac{1}{3}\left[\overset{(1)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j)\right]; \tag{2.44}$$

$$\overset{(1)}{\Phi}_{i_1,i_2}(0,k,m,j+1)=\Phi_{0,i_1,i_2}(k,m,j+1), \tag{2.45}$$

$$\overset{(1)}{\Phi}_{i_1,i_2}(N_1,k,m,j+1)=\overset{(1)}{\Phi}_{i_1,i_2}(N_1-1,m,j+1); \tag{2.46}$$

$$\frac{1}{3}\frac{\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\dot{\Phi}_{i_1,i_2}(i,k,m,j+1)}{\tau}=\frac{1}{h_2}\left\{k_{i,y}\left(i,k+\frac{1}{2},m,j+\frac{1}{2}\right)\times\frac{\overset{(2)}{\Phi}_{i_1,i_2}(i,k+1,m,j+1)-\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j+1)}{h_2}-\right.$$

$$\left.-k_{i_1,y}\left(i,k-\frac{1}{2},m,j+\frac{1}{2}\right)\times\frac{\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\overset{(2)}{\Phi}_{i_1,i_2}(i,k-1,m,j+1)}{h_2}\right\}\frac{1}{3}f_{i_1,i_2}\left(i,k,m,j+\frac{1}{2}\right),$$

$(k=1,2,..2N_2-1, h_2=\frac{\ell_2}{N_2}),\forall(i,m);$ (2.47)

$$\overset{(2)}{\Phi}_{i_1,i_2}(i,1,m,j+1)=\overset{(2)}{\Phi}_{i_1,i_2}(i,0,m,j+1); \tag{2.48}$$

$$\overset{(2)}{\Phi}_{i_1,i_2}(i,2N_2,m,j+1)=\overset{(2)}{\Phi}_{i_1,i_2}(i,2N_2-1,m,j+1); \tag{2.49}$$

$$\overset{\bullet}{\Phi}_{i_1,i_2}(i,k,m,j)=\frac{1}{3}\left[\overset{(1)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j)\right]; \tag{2.50}$$

$$\frac{1}{3}\frac{\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\overset{\bullet}{\Phi}_{i_1,i_2}(i,k,m,j)}{\tau}=\frac{1}{h_3}\left\{k_{i_1,z}\left(i,k,m+\frac{1}{2},j+\frac{1}{2}\right)\times\frac{\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m+1,j+1)-\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j+1)}{h_3}-\right.$$

$$\left.-k_{i_1,z}\left(i,k,m-\frac{1}{2},j+\frac{1}{2}\right)\times\frac{\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j+1)-\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m-1,j+1)}{h_3}\right\}-\frac{1}{3}f_{i_1,i_2}\left(i,k,m,j+\frac{1}{2}\right), \tag{2.51}$$

$(m=1,\ldots,N_3-1,\ h_3=\frac{\ell_3}{N_3}),\forall(i,k);$

$$\overset{(3)}{\Phi}_{i_1,i_2}(i,k,1,j+1)=\overset{(3)}{\Phi}_{i_1,i_2}(i,k,0,j+1); \tag{2.52}$$

$$\overset{(3)}{\Phi}_{i_1,i_2}(i,k,N_3,j+1)=\overset{(3)}{\Phi}_{i_1,i_2}(i,k,N_3-1,j+1); \tag{2.53}$$

$$\overset{\bullet}{\Phi}_{i_1,i_2}(i,k,m,j)=\frac{1}{3}\left[\overset{(1)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(2)}{\Phi}_{i_1,i_2}(i,k,m,j)+\overset{(3)}{\Phi}_{i_1,i_2}(i,k,m,j)\right]. \tag{2.54}$$

Additive finite-difference scheme of parallel calculation (2.41), (2.43)-(2.46), (2.47)-(2.50), (2.51)-(2.54) is absolutely stable and provides accuracy $O(\tau+h^2)$, $h^2=\sum_{i=1}^{3}h_i^2$.

For solution of the scheme the method of scrolling (a modified factorization method) is used.

Obtained in that way $s^{(1)}_{i_1,i_2}(i,k,m,j+1)$, $s^{(2)}_{i_1,i_2}(i,k,m,j+1)$, and $s^{(3)}_{i_1,i_2}(i,k,m,j+1)$, allow to construct the approximate value in grid nodes $\omega_h=\omega_x\times\omega_y\times\omega_z$ at moment t_{j+1} in the following way:

$$\Phi_{i_1,i_2}(x_i,y_k,z_m,t_{j+1})\approx\overset{\bullet}{\Phi}_{i_1,i_2}(i,k,m,j+1)=\frac{1}{3}\left[s^{(1)}_{i_1,i_2}(i,k,m,j+1)+s^{(2)}_{i_1,i_2}(i,k,m,j+1)+s^{(3)}_{i_1,i_2}(i,k,m,j+1)\right]$$

As it may be seen from the above, the obtained values $\overset{\bullet}{\Phi}_{i_1,i_2}(i,k,m,j+1)$ are taken as the initial condition for the $j+2$ th layer and so on.

Time T, i.e. the number of layers K, depends on the time grid interval and is chosen according to user requirements.

Note 1. In case of non-local boundary condition, instead of condition (2.46), is taken:

$$\Phi^{(1)}_{i_1,i_2}(N_1,k,m,j+1)=q.\Phi^{(1)}_{i_1,i_2}(\widetilde{i},k,m,j+1),\ (i=1,...,N_1-1),\ \forall(k,m), \tag{2.55}$$

where $\widetilde{i}=\left[\frac{\xi}{h_1}\right]$, $\left[\frac{\xi}{h_1}\right]$ is the integral part from division.

Of practical interest is the value of Φ_{i_1,i_2} at point (ξ,y,z,t), i.e. at a point within the controlled range. To find it, the following procedures are used:

either linear interpolation

$$\dot{\Phi}_{i_1,i_2}(\xi,y_k,z_m,t)=(\frac{\xi}{h_1}-(i^*-1)).\dot{\Phi}_{i_1,i_2}(i^*,y_k,z_m,t)+(i^*-\frac{\xi}{h_1}).\dot{\Phi}_{i_1,i_2}((i^*-1),y_k,z_m,t),$$

or a simple carry

$$\dot{\Phi}_{i_1,i_2}(\xi,y_k,z_m,t)\approx\dot{\Phi}_{i_1,i_2}\left(\left[\frac{\xi}{h_1}\right].h_1,y_k,z_m,t\right)$$

that has accuracy $O(h_1)$, x_{i^*-1}, x_{i^*} are the nearest grid nodes for ξ.

Note 2. In case of replacement of (2.46) with (2.55), a modification of the method of scrolling or of the factorization method is used.

2.6. Optimization Problems of the Algorithms Connected with Difference Schemes

Let us consider problems of optimum choice of the parameters of the algorithm at practical realization of difference schemes [38, 40]. As criterion of optimality, there is considered the necessity of maximum decreasing the computation time and error. Offered below algorithm is suitable for the case when the function describing the transfer of pollutants in water has derivatives including fourth order.

2.6.1. Optimization, Used in Boundary Problem

Let us consider the problem formulated in Item 2.1.1. Further are used designations introduced in appointed item.

1. Estimation of the misclosure in one-dimensional difference schemes. In one dimensional case, the misclosure of approximation of the equation, corresponding to the difference operator $\hat{\alpha}_h$ can be determined as follows: $\rho(x,h)=h^2\cdot\rho_h(x,h)$, where

$$\rho_h(x,h)=\frac{1}{24}\left(\frac{\partial}{\partial h'}\right)^4\left(G_{dn}(x,h')\cdot\Phi(x-h')+G_{md}(x,h')\cdot\Phi(x)+G_{up}(x,h')\cdot\Phi(x+h')\right);$$

h' is some number from the interval $(0,h)$.

Correct to the terms of order h^3, takes place $\rho(x,h)\approx h^2\cdot\rho_h(x,0)$, and

$$\rho_h(x,0)=-\frac{1}{12}A(x)\cdot\frac{d^4}{dx^4}\Phi(x)+\frac{1}{6}\widetilde{B}(x)\cdot\frac{d^3}{dx^3}\Phi(x)+$$
$$+U(x)\cdot\frac{d^2}{dx^2}\Phi(x)+\left(V_{up}(x,0)-V_{dn}(x,0)\right)\cdot\frac{d}{dx}\Phi(x).$$

If coefficients of the difference operator are determined by relation (2.1), then

$$\rho_h(x,0)=-\frac{1}{12}A(x)\frac{d^4}{dx^4}\Phi(x)+\frac{1}{6}\widetilde{B}(x)\frac{d^3}{dx^3}\Phi(x)-\frac{1}{8}\ddot{A}(x)\frac{d^2}{dx^2}\Phi(x)-\frac{1}{24}\dddot{A}\frac{d}{dx}\Phi(x).$$

At $A(x)=A=const$

$$\rho_h(x,0)=-\frac{1}{12}A\cdot\frac{d^4}{dx^4}\Phi(x)+\frac{1}{6}B(x)\cdot\frac{d^3}{dx^3}\Phi(x).$$

2. Estimation of the misclosure in multi-dimensional difference schemes. Let us consider m-dimensional boundary problem at the same conditions which were considered in Item 2 of Paragraph 1.3.1. In particular, tensor $A(x)$ is supposed to be diagonal. The latter condition means that the misclosure of the equation in this case can be presented in the form of the sum of m misclosures corresponding to different coordinate axes:

$$\rho(\boldsymbol{x},h)=\sum_{k=1}^{m}h_k^2\cdot\rho_k(\boldsymbol{x},h_k),$$

and, correct to the terms of order h^3, it is possible in the equation above to replace functions $\rho_k(\boldsymbol{x},h_k)$ with their values $\rho_k(\boldsymbol{x},0)$. Expressions for $\rho_k(\boldsymbol{x},h_k)$ and $\rho_k(\boldsymbol{x},0)$ for each value $k=1,...,m$ are similar to the corresponding expressions for the misclosures in the one-dimensional problem (in these expressions it is necessary to replace the scalar functions $A(x)$ and $B(x)$ with corresponding components $A_{kk}(\boldsymbol{x})$ and $B_k(\boldsymbol{x})$). In particular, at $A(\boldsymbol{x})=A=const$,

$$\rho_k(\boldsymbol{x},0) = -\frac{1}{12} A_{kk} \cdot \nabla_k^4 \Phi(\boldsymbol{x}) + \frac{1}{6} B_k(\boldsymbol{x}) \cdot \nabla_k^3 \Phi(\boldsymbol{x}).$$

3. Optimization of the choice of numbers $n_1,...,n_m$. The total number of nodal points N determines the time necessary for realization of the algorithm; the accuracy of the obtained result depends on it. Naturally, there arises the question: how it is necessary to pick up the numbers $n_1,...,n_m$ at the given value N so that the algorithm should be somewhat optimum.

In conformity with the stated above, the upper bound of the module of the misclosure $\left|\rho(\boldsymbol{x},h)\right|$ of the considered equation can be presented in the form of

$$\sum_{k=1}^{m} \rho_k \, h_k^2 ,$$

where $\rho_1,...,\rho_m = const$.

Let us introduce an auxiliary parameter

$$H = \prod_{k=1}^{m} h_k^2 = \left(\frac{V}{n_1 ... n_m} \right)^2 \approx \left(\frac{V}{N} \right)^2 ,$$

where

$$V \equiv \prod_{k=1}^{m} (b_k - a_k)$$

is the volume of the hyper parallelepiped limiting the region X.

The optimization consists in that, at the given value N (i.e. at the given value H), there are defined such values $h_1,...,h_m$ for which the upper bound of the module of the misclosure assumes the minimum value:

$$\begin{cases} \sum\limits_{k=1}^{m} \rho_k \, h_k^2 \to \min, \\ \prod\limits_{k=1}^{m} h_k^2 = H = \text{const}. \end{cases}$$

The solution of this optimization problem is determined by formulae:

$$h_k^2 = \frac{1}{\rho_k} \left(H \prod_{k=1}^{m} \rho_k \right)^{1/m} \qquad (k = 1,...,m). \tag{2.56}$$

Thus, at the optimum choice of spatial steps of the grid along different coordinate axes, the upper bound of the misclosure proves to be the sum of m equal components, each of which is proportional to the square of the corresponding step h_k. In other words, each of parameters h_k brings identical "contribution" to the error of the result.

The main difficulty for practical realization of the described scheme of optimization is the necessity of estimation of the upper bound of partial derivatives of function $\Phi(\boldsymbol{x})$ with respect to the spatial coordinates in terms of which parameters ρ_k are expressed (see Section 2.6.3) without solving the differential equation.

2.6.2. Optimization, Used at Solving Diffusion Equation

Let us consider the problem formulated in Item 2.1.2. Further are used designations introduced in appointed item.

1. Estimation of the misclosure. Let the difference operator $\hat{\alpha}_h(t)$ approximating $\hat{\alpha}(t)$ be known:

$$\hat{\alpha}_h(t)\,\Phi(t,\boldsymbol{x}) = \hat{\alpha}(t)\,\Phi(t,\boldsymbol{x}) + h^M\ \rho_h(\boldsymbol{x},t,h)\,.$$

The accuracy of approximation of the diffusion equation by the difference equation is characterized by misclosure $\rho(t,\boldsymbol{x},\tau,h)$:

$$\begin{aligned}&\frac{1}{\tau}\,D(t+\nu\tau,\boldsymbol{x})\cdot\big(\Phi(t+\tau,\boldsymbol{x})-\Phi(t,\boldsymbol{x})\big)+\\ &+\sigma\cdot\hat{\alpha}_h(t+\nu\tau)\,\Phi(t+\tau,\boldsymbol{x})+(1-\sigma)\cdot\hat{\alpha}_h(t+\nu\tau)\,\Phi(t,\boldsymbol{x})=\\ &\qquad=f(t+\nu\tau,\boldsymbol{x})+\rho(t+\nu\tau,\boldsymbol{x},\tau,h).\end{aligned}$$

The last equation is exact. It transforms into the difference equation which can be used for the approximate solution of the initial diffusion equation if we neglect the function ρ(...) in its right part.

The last equation can also be rewritten in the form of the equation for layers:

$$\hat{\alpha}_{lau}^{(h)}\ \Phi_{lau}(\boldsymbol{x}) = f_{lau}(\boldsymbol{x}) + \rho(t',\boldsymbol{x},\tau,h)\,,$$

where

$$\hat{\alpha}_{lau}^{(h)} = \sigma\cdot\hat{\alpha}_h(t') + \frac{1}{\tau}\,D(t',\boldsymbol{x})\cdot\hat{I};\qquad t' = t+\nu\tau\,.$$

For the symmetric scheme:

$$\rho(t, \boldsymbol{x}, \tau, h) = h^M \rho_h(t, \boldsymbol{x}, h) + \tau^2 \rho_\tau(t, \boldsymbol{x}, \tau, h),$$

where

$$\rho_\tau(t, \boldsymbol{x}, \tau, h) = \frac{1}{48} D(t, \boldsymbol{x}) \left(\Phi^{(3)}(t + \tau'/2, \boldsymbol{x}) + \Phi^{(3)}(t - \tau'/2, \boldsymbol{x})\right) +$$
$$+ \frac{1}{16} \hat{\alpha}_h(t) \left(\Phi^{(2)}(t + \tau''/2, \boldsymbol{x}) + \Phi^{(2)}(t - \tau''/2, \boldsymbol{x})\right);$$

τ' and τ'' are some numbers from the interval $(0, \tau)$; $\Phi^{(k)}(t, \boldsymbol{x}) \equiv (\partial / \partial t)^k \Phi(t, \boldsymbol{x})$.

The misclosure has the order $\tau^2 + h^M$.
Correct to the terms of order τ

$$\rho_\tau(t, \boldsymbol{x}, \tau, h) = \frac{1}{24} D(t, \boldsymbol{x}) \Phi^{(3)}(t, \boldsymbol{x}) + \frac{1}{8} \hat{\alpha}_h(t) \Phi^{(2)}(t, \boldsymbol{x}).$$

For all other schemes, except the symmetric one,

$$\rho(t, x, \tau, h) = h^M \rho_h(t, x, h) + \tau \rho_\tau(t, x, \tau, h),$$

where

$$\rho_\tau(t, \boldsymbol{x}, \tau, h) =$$
$$= \frac{1}{2} D(t, \boldsymbol{x}) \left((1-\nu)^2 \cdot \Phi^{(2)}(t + (1-\nu)\tau', \boldsymbol{x}) - \nu^2 \cdot \Phi^{(2)}(t - \nu\tau', \boldsymbol{x})\right) +$$
$$+ \hat{\alpha}_h(t) \left(\sigma(1-\nu) \cdot \Phi^{(1)}(t + (1-\nu)\tau'', \boldsymbol{x}) - \nu(1-\sigma) \cdot \Phi^{(1)}(t - \nu\tau'', \boldsymbol{x})\right);$$

τ' and τ'' are some numbers from the interval $(0, \tau)$; $\Phi^{(k)}(t, \boldsymbol{x}) \equiv (\partial / \partial t)^k \Phi(t, \boldsymbol{x})$.

The misclosure has the order $\tau + h^M$.
Correct to the terms of order τ

$$\rho_\tau(t, \boldsymbol{x}, \tau, h) = (1/2 - \nu) D(t, \boldsymbol{x}) \Phi^{(2)}(t, \boldsymbol{x}) + (\sigma - \nu) \hat{\alpha}_h(t) \Phi^{(1)}(t, \boldsymbol{x}).$$

2. Optimization of the choice of parameter τ for the scheme of the τ^2 order. Similarly to the solution of boundary problems, at realization of difference schemes for the diffusion equation, the question arises: how to pick up the parameters of the algorithm in the optimum way. In this case, it is the question of the optimum choice of the parameter τ at the given spatial steps of the grid.

We shall consider that the mean time it takes the computer to solve the set of N linear equations at big values of N is proportional to N^k, where k is some positive constant.

If the method of scrolling is used at solution of the set of equations, then $k \approx 1$.

If the Seidel method is used at solution of the set of equations and the number of nonzero elements in each row of the matrix of the considered set is fixed and does not depend on N, then $k \approx 1$.

Let the operator $\hat{\alpha}$ be determined by relation (2.6), where functions $C(\boldsymbol{x})$, $B(\boldsymbol{x})$ and $A(\boldsymbol{x})$ satisfy the same conditions as in the previous Section; in particular, the tensor $A(\boldsymbol{x})$ should be diagonal.

In conformity with the stated above in the present and previous Sections, when the symmetric difference scheme is used, the upper bound of the module of the misclosure $|\rho(t, \boldsymbol{x}, \tau, h)|$ of the considered diffusion equation can be presented in the form of

$$\rho_\tau \, \tau^2 + \sum_{k=1}^{m} \rho_k \, h_k^2 ,$$

where $\rho_\tau, \rho_1, ..., \rho_m = const$. Here we use the same designations as in Item 3 of the previous Section; in particular, h_k is the step of the grid along the k-th coordinate axis. The values of parameters h_k we shall determine by formulae (2.56):

$$\rho_k \, h_k^2 = \frac{1}{m} P \cdot N^{-2/m} ,$$

where $P \equiv m \cdot (\rho_1 ... \rho_m)^{1/m} \cdot V^{2/m}$.

The time necessary for calculation of the layers of function $\Phi(t, \boldsymbol{x})$ with numbers $0,1,...,K$ at fixed value $t = K\tau$ is proportional to N^k / τ.

The optimization consists in that, at the given value of upper bound of the module of the misclosure of the equation which is equal to ε, there are defined such values τ and N for which the time of calculation assumes the minimum value:

$$\begin{cases} N^\kappa / \tau \to \min, \\ \rho_\tau \, \tau^2 + P \, N^{-2/m} = \varepsilon = \text{const}. \end{cases}$$

The solution of this optimization problem is determined by formulae:

$$N = \left(\frac{P(\kappa + 1/m)}{\kappa \varepsilon} \right)^{m/2}; \qquad \tau^2 = \frac{1}{\rho_\tau} \frac{\varepsilon}{1 + \kappa m};$$

$$\rho_1 h_1^2 = ... = \rho_m h_m^2 = \kappa \rho_\tau \tau^2 = \frac{\kappa\varepsilon}{1+\kappa m}.$$

In the case when $k = 1$, at the optimum choice of spatial steps of the grid and the step of digitization of the time, the upper bound of the misclosure proves to be the sum of $m + 1$ equal components, each of which depends only on one of the parameters: $\tau, h_1, ..., h_m$. This result is similar to the one obtained in Item 3 of the previous Section.

The main difficulty in practical realization of the described scheme of optimization, as well as in realization of the similar scheme at solution of the boundary problem, is the necessity in estimation of the upper bound of partial derivatives of the function $\Phi(t, \boldsymbol{x})$ by time and spatial coordinates in terms of which parameters ρ_τ and ρ_k are expressed (see Section 2.6.3) without solving the diffusion equation.

3. Optimization of the choice of parameter τ for the scheme of the τ order. Let us consider the same problem as in the previous Item provided that the used difference scheme is not symmetric. In this case, the upper bound of the module of the misclosure $|\rho(t, \boldsymbol{x}, \tau, h)|$ of the considered diffusion equation can be presented in the form of

$$\rho_\tau \tau + \sum_{k=1}^{m} \rho_k h_k^2,$$

where $\rho_\tau, \rho_1, ..., \rho_m = const$.

We can repeat all the stated in the previous Item with minor amendments. The condition of optimization is written in the form of

$$\begin{cases} N^\kappa / \tau \to \min, \\ \rho_\tau \tau + P N^{-2/m} = \varepsilon = \text{const}. \end{cases}$$

The solution of this optimization problem is determined by formulae:

$$N = \left(\frac{P(\kappa + 2/m)}{\kappa\varepsilon} \right)^{m/2}; \qquad \rho_\tau \tau = \frac{\varepsilon}{1+\kappa m/2};$$

$$\rho_1 h_1^2 = ... = \rho_m h_m^2 = \frac{1}{2}\kappa \rho_\tau \tau^2 = \frac{\varepsilon\kappa/2}{1+\kappa m/2}.$$

2.6.3. Estimation of Unknown Function Derivatives

As already mentioned in the previous two sections, for practical realization the described optimization schemes, it is necessary to estimate somehow the upper bounds of the modules

of partial derivatives of the unknown function with respect to independent variables without solving the boundary or the mixed problem.

It should be borne in mind that the derivatives of these functions can be estimated up to the common constant multiplier.

One of the ways of the solution of this problem consists in the following: for some values of the parameters h_k and τ (at solution of diffusion equation), the values of the function Φ are determined as a first approximation, then, by means of the numerical differentiation operations the required derivatives are determined and the values of the sought for the parameters are calculated. After that, using these values there are determined new values of the function Φ and so on until the difference between the neighbouring calculated values of the function are less than the given value. At the solution of the diffusion equation it is possible to use the explicit scheme at the first stage. Further it is necessary to determine the values of the sought function with higher accuracy.

In this case, for calculation of the unknown function values, there is applied the iteration method similar to the one used in work [1, 44, 45] at calculation of the multidimensional integral by the Monte-Carlo method, at calculation of estimations of the polynomial regression on the basis of active experiment and at calculation of the covariance function with given accuracy.

It is known that the operations of numerical differentiation are not steady, but this should not prevent the realization of the offered method which is effected in the package of realization of mathematical models of pollutants transfer in rivers (see Chapter 6) since it requires only the rough estimates of unknown derivatives.

The obvious draw-back of the given method is necessity of performance of a plenty of additional actions.

2.6.4. Examples of Using of the Offered Optimization

Let us bring the control examples with the use of the described optimization of choosing the parameters [38, 40].

1. Boundary problem. Let us consider the function of two variables:

$$\Phi^{ex}(x_1, x_2) \equiv \left(u_1 \cdot e^{\lambda_1 x_1} + v_1 \cdot e^{\mu_1 x_1}\right)\left(u_2 \cdot e^{\lambda_2 x_2} + v_2 \cdot e^{\mu_2 x_2}\right),$$

where $\lambda_1, \mu_1, u_1, v_1, \lambda_2, \mu_2, u_2, v_2 = const$. This function satisfies the homogeneous equation with constant coefficients:

$$\left(-A_1 \nabla_1^2 - A_2 \nabla_2^2 + B_1 \nabla_1 + B_2 \nabla_2 + C\right) \Phi^{ex}(x_1, x_2) = 0,$$

where A_1 and A_2 are the arbitrary constants;

$$B_1 = A_1(\lambda_1 + \mu_1); \quad B_2 = A_2(\lambda_2 + \mu_2);$$

$$C = -A_1\lambda_1\mu_1 - A_2\lambda_2\mu_2 .$$

In the considered control examples, the function $\Phi^{ex}(x_1, x_2)$ is considered as the solution of the boundary problem for the rectangular region which is assigned by conditions:

$$a_1 \le x_1 \le b_1; \quad a_2 \le x_2 \le b_2,$$

with boundary conditions:

$$(p_1' + q_1' \nabla_1)\,\Phi(\boldsymbol{x})\big|_{x_1=a_1} = \psi_1'(x_2); \qquad (p_1'' + q_1'' \nabla_1)\,\Phi(\boldsymbol{x})\big|_{x_1=b_1} = \psi_1''(x_2);$$
$$(p_2' + q_2' \nabla_2)\,\Phi(\boldsymbol{x})\big|_{x_2=a_2} = \psi_2'(x_1); \qquad (p_2'' + q_2'' \nabla_2)\,\Phi(\boldsymbol{x})\big|_{x_2=b_2} = \psi_2''(x_1),$$

where $p_1', q_1', p_1'', q_1'', p_2', q_2', p_2'', q_2''$ are the arbitrary constants; $\psi_1'(x_2), \psi_1''(x_2), \psi_2'(x_1), \psi_2''(x_1)$ are functions, the expressions for which can be obtained by means of the substitution of the expression for $\Phi^{ex}(x_1, x_2)$ into the boundary conditions.

The function $\Phi^{ex}(x_1, x_2)$ values are compared to the numerical calculation results. The initial data in the considered problem are the following.

The parameters which determine the boundaries of the region are:

$$a_1 = -1; \; b_1 = 5; \; a_2 = -0.5; \; b_2 = 3.5.$$

The parameters which determine the boundary conditions (Dirichlet condition) are:

$$p_1' = p_1'' = p_2' = p_2'' = 1; \qquad q_1' = q_1'' = q_2' = q_2'' = 0.$$

The equation coefficients and the function $\Phi^{ex}(x_1, x_2)$ parameters are:

$A_1 = 1.0;$	$A_2 = 1.0$;		
$B_1 = 0.0$;	$B_2 = 0.30$;	$C = 6.08$;	
$u_1 = 0.00045$;	$v_1 = 3.11270$;	$\lambda_1 = 2.0$;	$\mu_1 = -2.0$;
$u_2 = 0.02562$;	$v_2 = 6.78059$;	$\lambda_2 = 1.6$;	$\mu_2 = -1.3$.

The minimum and maximum values of the required function in the considered region are:

$y_{min} = 0.083$; $\qquad y_{max} = 299.0$.

The numerical calculations are performed in two ways: without optimization and with optimization of the choice of numbers n_1 and n_2, described in Item 3 of Section 2.6.1. In

both cases, the total number of nodal points is accepted equal to $N \approx 1000$.

At carrying out the calculations without optimization, the numbers n_1 and n_2 are selected so that spatial steps of the grid h_1 and h_2 were approximately equal. As a result we have:

$h_1 = 0.162$; $h_2 = 0.167$; $n_1 = 37$; $n_2 = 24$.

In this case, the maximum deviation of the calculated values of the desired function from its exact values is equal to

$$\max\{\Delta y_i\} = 3.24.$$

At carrying out the calculations with optimization, at first we put $n_1 = n_2 = 15$, determine the initial estimate of the values of the desired function, then we determine the optimum values of parameters ρ_1 and ρ_2 and carry out more exact calculations corresponding to the obtained values ρ_1 and ρ_2 and $N \approx 1000$. As a result, we have:

$\rho_1 = 44.6549$; $\rho_2 = 9.21596$;

$h_1 = 0.107$; $h_2 = 0.250$; $n_1 = 56$; $n_2 = 16$.

In this case, the maximum deviation of the calculated values of the desired function from its exact values is equal to

$$\max\{\Delta y_i\} = 1.018.$$

The calculation time slightly increases at optimization. For the considered case – approximately 1.2 times (for example at using Pentium-IV, the calculation time of the given example without optimization is equal to 0.13 s, and with optimization – to 0.16 s).

Thus, the use of optimization leads to a significant increase in the accuracy of the results at a slight increase in the time of calculation.

2. Diffusion equation. Let us consider the function of three variables:

$$\Phi^{ex}(t, x_1, x_2) \equiv \left(u_1 \cdot e^{\lambda_1 x_1} + v_1 \cdot e^{\mu_1 x_1}\right)\left(u_2 \cdot e^{\lambda_2 x_2} + v_2 \cdot e^{\mu_2 x_2}\right) \cdot e^{-st},$$

where $\lambda_1, \mu_1, u_1, v_1, \lambda_2, \mu_2, u_2, v_2, s = const$. This function satisfies the homogeneous diffusion equation with constant coefficients:

$$D \frac{\partial}{\partial t} \Phi^{ex}(t, x_1, x_2) + \\ + \left(-A_1 \nabla_1^2 - A_2 \nabla_2^2 + B_1 \nabla_1 + B_2 \nabla_2 + C\right) \Phi^{ex}(t, x_1, x_2) = 0,$$

where D, A_1 и A_2 are the arbitrary constants;

$$B_1 = A_1(\lambda_1 + \mu_1); \quad B_2 = A_2(\lambda_2 + \mu_2);$$
$$C = Ds - A_1\lambda_1\mu_1 - A_2\lambda_2\mu_2.$$

In the considered control examples, the function $\Phi^{ex}(t, x_1, x_2)$ defined at $t \geq 0$ and

$$a_1 \leq x_1 \leq b_1; \quad a_2 \leq x_2 \leq b_2,$$

is considered as the solution of the mixed problem, which includes the diffusion equation, the initial condition

$$\Phi(0, \boldsymbol{x}) = \Phi_0(\boldsymbol{x}) \equiv \left(u_1 \cdot e^{\lambda_1 x_1} + v_1 \cdot e^{\mu_1 x_1}\right)\left(u_2 \cdot e^{\lambda_2 x_2} + v_2 \cdot e^{\mu_2 x_2}\right)$$

and the boundary conditions:

$$(p_1' + q_1' \nabla_1)\,\Phi(t, \boldsymbol{x})\big|_{x_1 = a_1} = \psi_1'(t, x_2); \quad (p_1'' + q_1'' \nabla_1)\,\Phi(t, \boldsymbol{x})\big|_{x_1 = b_1} = \psi_1''(t, x_2);$$

$$(p_2' + q_2' \nabla_2)\,\Phi(t, \boldsymbol{x})\big|_{x_2 = a_2} = \psi_2'(t, x_1); \quad (p_2'' + q_2'' \nabla_2)\,\Phi(t, \boldsymbol{x})\big|_{x_2 = b_2} = \psi_2''(t, x_1),$$

where $p_1', q_1', p_1'', q_1'', p_2', q_2', p_2'', q_2''$ are the arbitrary constants; $\psi_1'(t, x_2), \psi_1''(t, x_2), \psi_2'(t, x_1), \psi_2''(t, x_1)$ are the functions, the expressions for which can be obtained by means of substitution of the expression for $\Phi^{ex}(t, x_1, x_2)$ into the boundary conditions.

The function $\Phi^{ex}(t, x_1, x_2)$ values are compared to the numerical calculation results. The initial data in the considered problem are the following.

The parameters which determine the boundaries of the region are:

$$a_1 = -1; \; b_1 = 5; \; a_2 = -0.5; \; b_2 = 3.5.$$

The parameters which determine the boundary conditions (Dirichlet condition) are:

$$p_1' = p_1'' = p_2' = p_2'' = 1; \quad q_1' = q_1'' = q_2' = q_2'' = 0.$$

The equation coefficients and the function $\Phi^{ex}(t, x_1, x_2)$ parameters are:

$$A_1 = 1.50; \qquad A_2 = 3.50;$$

$B_1 = 0.75$; $B_2 = 1.05$; $C = 16.28$; $D = 0.75$;
$u_1 = 0.000045$; $v_1 = 3.11271$; $\lambda_1 = 2.5$; $\mu_1 = -2.0$;
$u_2 = 0.02562$; $v_2 = 6.78059$; $\lambda_2 = 1.6$; $\mu_2 = -1.3$.
$s = 2.0$.

Minimum and maximum values of the function $\Phi_0(\boldsymbol{x})$ in the considered region are:

$$y_{\min} = 0.0446; \qquad y_{\max} = 299.0.$$

The number

$$\tau_0 = \frac{D/2}{A_1/h_1^2 + A_2/h_2^2},$$

which is approximately equal to the upper bound of the parameter τ, at which the explicit scheme of the diffusion equation solution is stable, is considered as a "standard" of the step of digitization of the time; concrete values of the parameter τ may be compared with τ_0. The choice of a smaller value of the "standard" accomplishes nothing except for a senseless increase in the calculation time. Especially, as it is evident from the further discussion the optimum value of the parameter τ is much bigger than τ_0.

The numerical calculations are performed in two ways: without optimization and with optimization of choosing the parameter τ, described in Section 2.6.2. In both cases, the total number of nodal points is accepted equal to $N \approx 1000$. In this case,

$h_1 = 0.12766$; $h_2 = 0.21053$; $n_1 = 47$; $n_2 = 19$.

The specified values h_1 and h_2 are obtained by means of the algorithm of optimization of the choice of spatial and time steps of digitization in the difference scheme of the diffusion equation solution. The algorithm is given below. Thus, in both cases, in the difference schemes the values of spatial steps of the grid are identical, and the corresponding algorithms are compared with each other only by the effect of the choice of the step of the time digitization.

At carrying out of calculations without optimization, we put $\tau = \tau_0$; the given parameter proves to be equal to $\tau = 0.00219$. The corresponding results of calculations for different values of t are given in Table 2.1-a.

At carrying out the calculations with optimization, at first we adopt $\tau = \tau_0$ and $n_1 = n_2 = 15$, determine the initial estimate of the values of the desired function for the layers with numbers $k = 0,...,8$, by means of the explicit scheme, then we determine the optimum values of the parameters ρ_τ, ρ_1 and ρ_2 and carry out more exact calculations

corresponding to the obtained values ρ_τ, ρ_1 and ρ_2 and $N \approx 1000$. As a result, the step of the time digitization proves to be equal to $\tau = 0.01370$; the corresponding results of calculations for different values of t are given in Table 2.1-b.

As is evident from the tables, the use of optimization leads to that the accuracy of calculations remains practically the same, and the time of calculations is reduced significantly.

Undoubtedly, there are also other methods of estimation of the parameters ρ_k and ρ_τ. This is the subject of further research, especially, as it is evident from the example, this considerably improves the calculation results of different schemes.

Table 2.1. The results of the numerical solution of the diffusion equation: a) without optimization; b) with optimization of the choice of the parameter τ

a)

k	t_k	$\max\{\Delta y_j\}$	$\max\{\Delta y_j/y_j\}$	T
322	0.71	0.40472	0.04063	16.69 s
644	1.41	0.09859	0.04028	15.38 s
966	2.12	0.02402	0.03910	14.11 s
1288	2.82	0.00585	0.03890	12.52 s

b)

k	*tk*	*max{□□yj}*	*max{□□yj/yj}*	*T*
52	*0.71*	*0.39964*	*0.03965*	*6.16 s*
104	*1.42*	*0.09613*	*0.03840*	*5.49 s*
156	*2.14*	*0.02312*	*0.03635*	*4.78 s*
208	*2.85*	*0.00556*	*0.03134*	*4.17 s*

The following values are given: k - the number of the layer (takes values K, $2K$, $3K$ and $4K$, where K is some natural number); t_k - the corresponding value of the variable t; $\max\{\Delta y_j\}$ and $\max\{\Delta y_j / y_j\}$ - the maximum absolute and relative deviations of the calculated values of the desired function from its exact values; T – the calculation time for the last K layers.

2.7. THE EFFECT OF SMOOTHNESS OF THE INHOMOGENEOUS PART OF THE DIFFUSION EQUATION ON THE ACCURACY OF THE RESULTS

Let the dynamics of propagation of the concentration of polluting substances in some section of the river be investigated by means of models described in Paragraph 1.2. The considered section of the river contains the point sources of pollution functioning continuously or for the limited time interval. It means that inhomogeneous parts of the solved diffusion equations contain the impulse functions, which are linear combinations of Dirac's delta-functions. These functions and their derivatives are not bounded. Therefore the difference schemes of the solution of diffusion equations are not correct in the vicinities of pollution source localization points.

Let us consider the problem of optimum choice of kinds of functions representing a non-uniform parts of diffusion equation at practical realization of difference schemes [40]. In addition as criteria of optimality, as well as in the previous paragraph, the necessity of maximum decrease in the error of calculation is considered. Furthermore chosen functions should be simple enough for realization, and they should correspond to real physical conditions as much as possible.

For elimination of this drawback, it is necessary to consider a model, in which the delta function $\delta(x-a)$ is replaced by the bounded numerical function $D(u,x-a)$, where u is the additional parameter. It means that the point sources are replaced by extended ones the capacity of each of which has the maximum corresponding to the capacity of the source at the point of its localization. Such sources can be named *quasi-point sources*.

The function $D(u,x)$ must satisfy the following requirements: it reaches the maximum value proportional to $1/u$ at the point $x=0$; it tends to zero at $x \to \pm\infty$; its integral between the limits $-\infty$ and $+\infty$ is equal to unit; its plot represents a bell-shaped curve. The width of such a curve is naturally defined as the width of the rectangle which height is equal to the ordinate of the peak of the curve, and its area is equal to the area of the figure limited by the curve and the axis of abscissas. Thus, the parameter u characterizes the width of the plot of the function $D(u,x)$, i.e. the sizes of the source. At $u \to 0$, the function $D(u,x)$ tends to $\delta(x)$.

One of the elementary functional dependences satisfying the listed requirements is the rectangular dependence:

$$D(u,x)=\begin{cases} 1/u & \text{at } |x| \le u/2, \\ 0 & \text{at } |x| > u/2. \end{cases}$$

However, the use of such dependence in practice is inexpedient, because the result of calculation of the values of such a function in the vicinity of the discontinuity point may be any of two numbers differing much from each other; this results from inevitable round-off errors of the values of the argument of the function. As shows the operational experience, this can lead to a curious situation when, for example, the function $D(u,x)$ is distinct from zero only in one of the cells into which nodal points divide the area X, but the computer program also determines nonzero values of this function for the neighbouring cell. Therefore, the same source of pollution will be counted twice, and the obtained result will be twice as much as the value which it should have.

It is possible to avoid the similar difficulty by means of using the continuous functional dependence for setting of $D(u,x)$, for example, it may be the trapezoid dependence:

$$D(u,x)=\begin{cases} 1/u & \text{at } t<1-s, \\ (1+s-t)/(2us) & \text{at } 1-s \le t \le 1+s, \\ 0 & \text{at } t>1+s, \end{cases}$$

where $t = 2|x|/u$; s is any real parameter from the interval $(0,1)$. The plot of this function together with the axis of abscissas forms an isosceles trapezium, the top and bottom bases of which have the lengths equal to $u(1-s)$ and $u(1+s)$, respectively, and the height of which is equal to $1/u$. The less is value s, the less differs this trapezium from a rectangle.

In the developed software package, besides the trapezoid dependence, the following dependences are offered to the user's choice:

1) Gaussian $$D(u,x) = \frac{1}{u\sqrt{2\pi}} e^{-\frac{1}{2}(x/u)^2};$$

2) Lorenzian $$D(u,x) = \frac{2}{2\pi u\left(1+(x/u)^2\right)}.$$

In fact, the function $D(u,x)$ defined by one of the two latter relations plays the part of a smoothing function, which allows us to transform any function from L^2 into an infinitely differentiable function by means of the operation of convolution [46].

If pollution sources do not operate continuous, but for a limited interval of time $[0,T]$, then the capacity of each source should be smoothed not only by spatial coordinates, but also by time. It means that this function should be proportional to $A(v,t-T)$, where v is the additional parameter, and $A(v,t)$ is the function satisfying the following conditions: at $t \to -\infty$ it tends to unit, and at $t \to +\infty$ - to zero. Its plot represents a quasi-stepped curve, which steepness is maximum at $t = 0$, and this maximum value of the steepness is proportional to $1/v$. The parameter v characterizes the time of diminution of the function of discharge. At $v \to 0$, the function $A(v,x)$ tends to $\vartheta(x)$, where $\vartheta(x)$ is Heaviside's stepped function. In the developed software package (see Chapter 6), there is possible the choice of an explicit form of the function $A(v,x)$ from the following types:

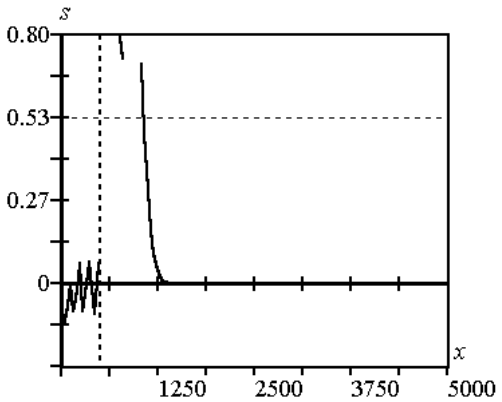
1) $$A(v,x) = \int_{t/v}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\tau^2/2} d\tau;$$

2) $$A(v,x) = \frac{1}{2} - \frac{1}{\pi}\arctan(t/v).$$

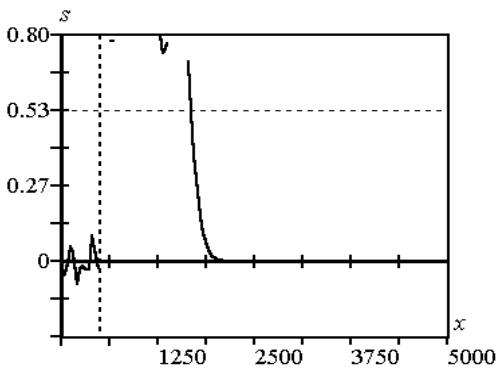
As shown the results of calculations (see below), the more smooth are the functions of discharge, the more exact are the results of solution of the equations in the vicinities of the points of discharge. For given types of function $D(u,x)$ and $A(v,x)$, the accuracy of the results increases at increasing of the values of parameters u and v.

The plots of the dependence of the calculated values of concentration s of the polluting substance from the x-coordinate at different moments of time t to which there correspond different numbers of steps k are presented in Figures 2.1-2.5. The function s is determined

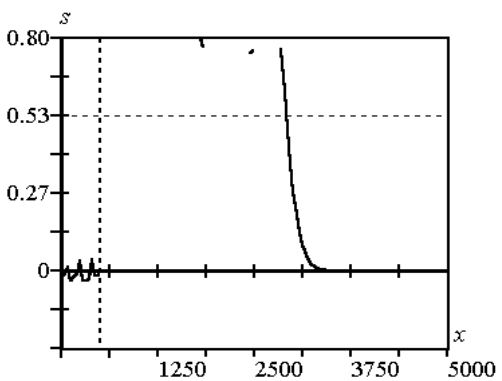
as a numerical solution of the one-dimensional diffusion equation under given zero, initial and boundary conditions for a rectangular section of the river in which a quasi-point source of pollution functions; there is supposed that the velocity of the flow is directed along the axis of abscissas.



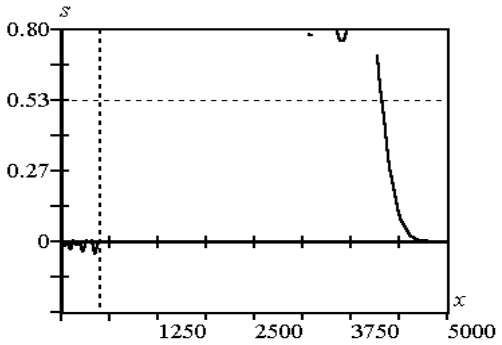
a) $t = 20$ min 44.98 s ($k = 31$);



b) $t = 41$ min 29.96 s ($k = 62$);

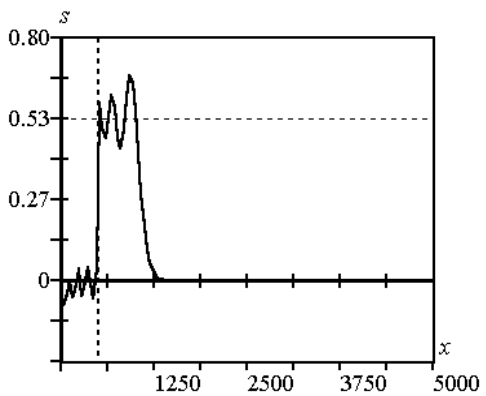


c) $t = 1$ h 22 min 59.92 s ($k = 124$);

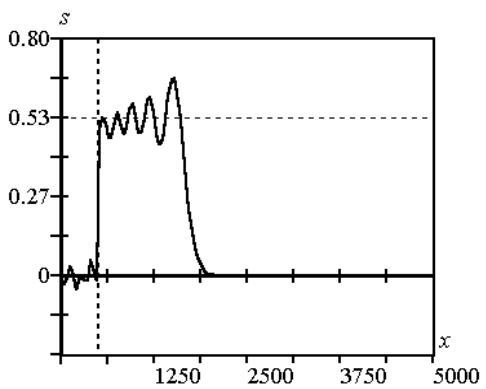


d) t = 2 h 04 min 29.88 s (k = 186).

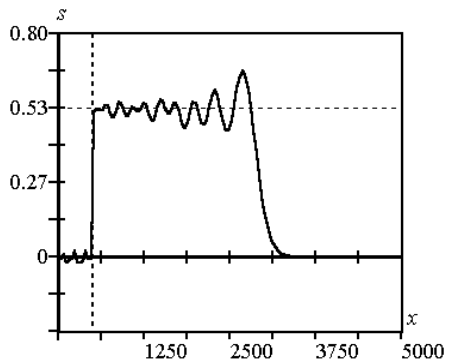
Figure 2.1. Plots of the polluting substance concentration in the rectangular section of the river in relation to the longitudinal coordinate x at $n = 250$; $\tau = 40.1606$; $u = 1.2$.



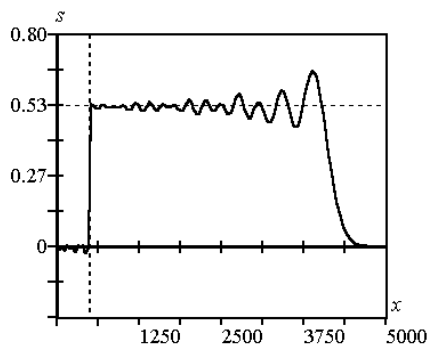
a) t = 20 min 44.98 s (k = 31);



b) t = 41 min 29.96 s (k = 62);

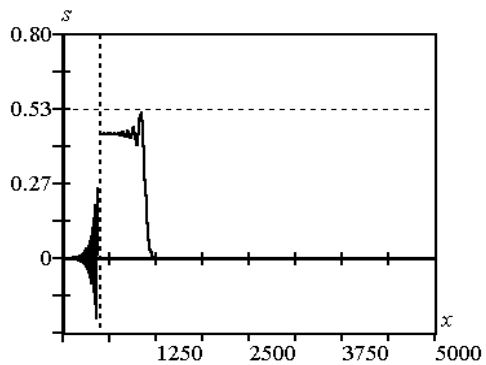


c) t = 1 h 22 min 59.92 s (k = 124);

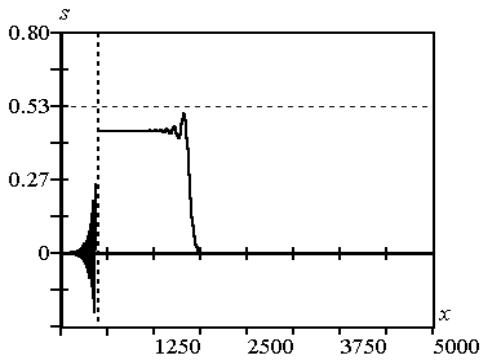


d) t = 2 h 04 min 29.88 s (k = 186).

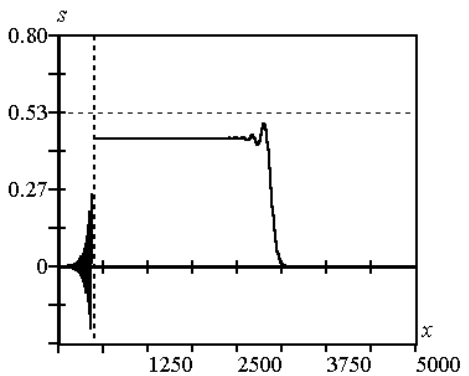
Figure 2.2. Plots of the polluting substance concentration in the rectangular section of the river in relation to the longitudinal coordinate x at $n = 250$; $\tau = 40.1606$; $u / h = 2$.



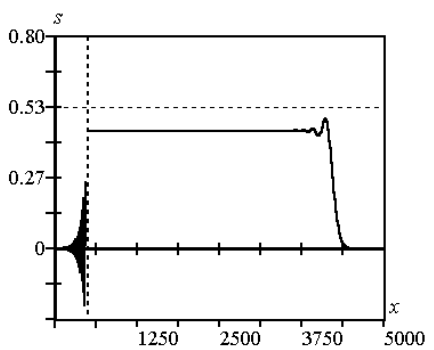
a) t = 20 min 51.25 s (k = 125);



b) t = 41 min 42.50 s (k = 250);

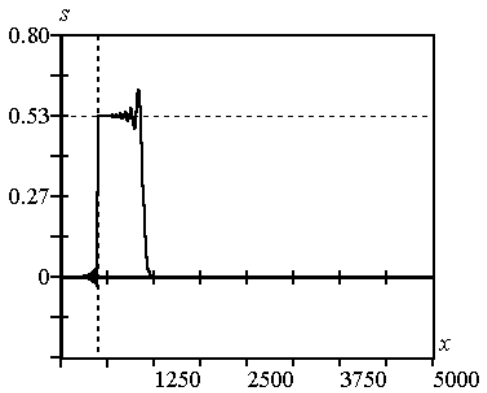


c) t = 1 h 23 min 25.00 s (k = 500);

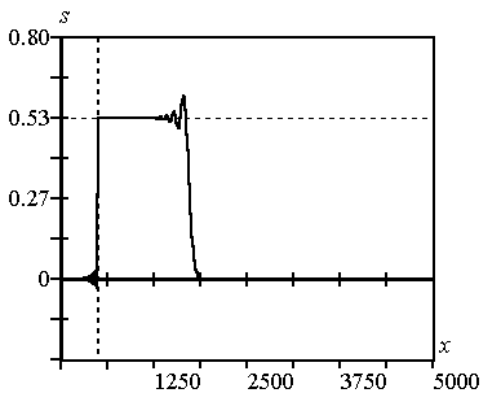


d) t = 2 h 05 min 7.51 s (k = 750).

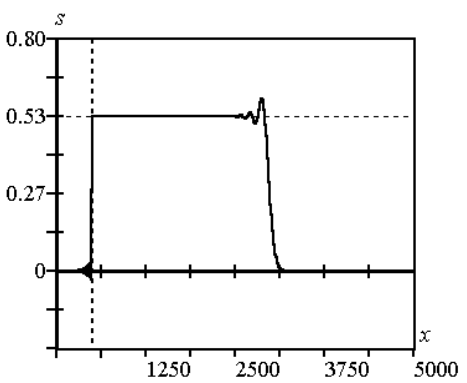
Figure 2.3. Plots of the polluting substance concentration in the rectangular section of the river in relation to the longitudinal coordinate x at $n = 1000$; $\tau = 10.0100$; $u/h = 1.2$.



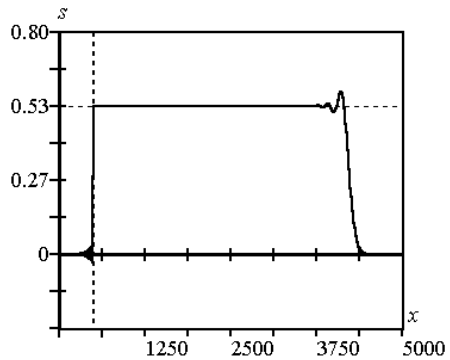
a) $t = 20$ min 51.25 s ($k = 125$);



b) $t = 41$ min 42.50 s ($k = 250$);

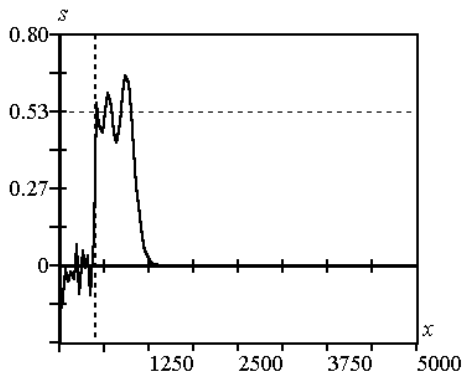


c) $t = 1$ h 23 min 25.00 s ($k = 500$);

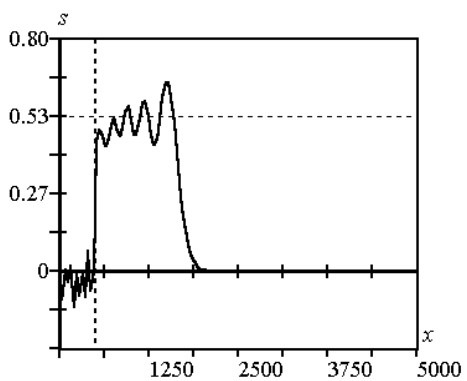


d) t = 2 h 05 min 7.51 s (k = 750).

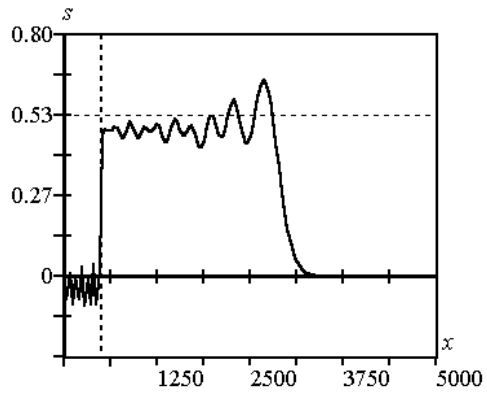
Figure 2.4. Plots of the polluting substance concentration in the rectangular section of the river in relation to the longitudinal coordinate x at $n = 1000$; $\tau = 10.0100$; $u/h = 2$.



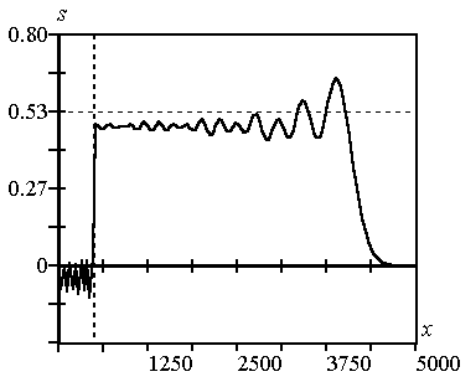
a) t = 20 min 44.98 s (k = 31);



b) t = 41 min 29.96 s (k = 62);



c) t = 1 h 22 min 59.92 s (k = 124);



d) t = 2 h 04 min 29.88 s (k = 186).

Figure 2.5. Plots of the polluting substance concentration in the rectangular section of the river in relation to the longitudinal coordinate x at $n = 250$; $\tau = 40.1606$; $u / h = 1.2$ and the Gaussian form of the function $D(u, x)$.

The initial data of the task are the following. The length of the section: $L = 5000$ m; the area of the cross-section: $E = 150$ m^2; the velocity of the flow: $v = 0.5$ m/s; the coordinate of the source of pollution: $x_q = 500$ m; the capacity of the source: $F = 40$ g/s; the diffusion factor: $K = 0.18$ m^2/s; the non-conservatism factor: $k = 0$.

Besides, different values of the following parameters correspond to different plots: the total number of nodal points n, the step of time digitization τ, and the quotient of the sizes of the source u and the spatial step of the grid h.

The oscillations of the obtained solutions, which are caused by their inaccuracy, are visible in the figures. Such oscillations, in particular, lead to that, at some points in the vicinities of the points of discharge, the obtained values of concentration proved to be negative, which is absurdity from the physical point of view.

The Gaussian form of the function $D(u, x)$ corresponds to the plots in Figure 2.5; the

rectangular form of this function $D(u,x)$ corresponds to the other plots. As shown in the figures, at $n=250$ and $u/h=1.2$, the plots corresponding to the rectangular and Gaussian forms of the function $D(u,x)$, differ essentially from each other. At $n=1000$ and/or $u/h=2$, practically identical plots correspond to rectangular and Gaussian forms of the function $D(u,x)$.

Considering this fact and comparing the corresponding plots in different figures, it is possible to draw the following conclusions:

- the accuracy of calculations considerably increases as the values of the source sizes divided by the spatial step of the grid increase;
- in the case of relatively small values n, the accuracy also increases at replacement of piece-smooth function $D(u,x)$ with the continuous-differentiable function;
- the increase in the accuracy of solutions, in particular, leads to smoothing of their oscillations.

For the two-dimensional model, the corresponding calculations give a similar results.

Up to this point we have considered the case when the section of the river has the rectangular form, and the diffusion factor, the non-conservatism factor and the velocity of the flow are constant in all sections. As a result, the coefficients of the diffusion equation prove to be constants. If the river banks are indented, then the coefficients of the equation prove to be oscillating piece-smooth functions of spatial coordinates. In the plots, analogous to the ones shown in Figure 2.1-2.5, constructed for a section of the river with “saw-tooth” banks, the oscillations of the obtained solutions are more considerable, especially in the case of relatively small values n.

The dependence of the accuracy of the solutions of the diffusion equation on the degree of smoothness of the coefficients of this equation and its inhomogeneous part can be explained as follows. It is known [47] that, if these functions are continuous (even if they are not continuous-differentiable), the solution of the equation is a two-time continuous-differentiable function. However, as shown in Section 2.1.1, the misclosure of the difference scheme on which the accuracy of the obtained solution depends, is proportional to the 4-th derivative of the unknown function with respect to spatial coordinates for which, under the considered conditions, the continuity is not guaranteed at all. If the coefficients of the equation are constant, its solution is an infinitely differentiable function, and, hence, the accuracy of the calculated values proves to be higher.

Chapter 3

STOCHASTIC MATHEMATICAL MODELS DESCRIBING POLLUTION OF THE RIVERS

The developed by authors methods of identification of statistical models, used at solving problems of studying and analysis of the quality of river's water and different problems of many areas of knowledge, are considered in this chapter.

3.1. STATISTICAL MODELS OF POLLUTANTS TRANSPORT IN THE RIVERS

The identification of statistical models as regression dependences is actual problem of mathematical statistics, arising at experimental data processing for quantitative description of unknown dependences among observed variables. It has numerous applications in many different areas of the science and practice, being irreplaceable means for quantitative description of cause and effect relations. Many activities are dedicated to the solution of this problem. Among them we shall note the following [1, 44, 45, 48-75, 131]. The problems of identification for different regression models are reviewed in these works: classical regression, regression at active and passive experiments. The algorithms with taking into account the stationarity or nostationarity of random components, presence or absence of correlation between them, the robustness of estimations are designed. The methods used in each of them are adapted to the features of a concrete problem and, despite of the optimality in a considered particular case, are poorly suitable in other conditions.

3.1.1. Statistical Models of Propagation of Pollutants in the Rivers

The essence of development of statistical models for description of transport of pollution substances in the rivers can be illustrated by such example [1, 76]. Let's split controled water object on $J-1$ sections by J controled cross-sections. Let's consider one of these sections. Let controled j th section of the water object is exposed of influence of p_j concentrated controled sources of pollution. In discrete moments of time $n=1,...,N$, in controled cross-

sections and areas of effect of pollution sources, the concentrations $C_{ip}(n)$ of i th ingredients and expenses of water masses $Q_p(n), p = 1,..., p_j$ are measured. The influence of other pollution factors on water quality is taken into account by some discrete function $v_{ij}(n)$. Let's designate by $q_{ip} = C_{ip}Q_p, p = 1,..., p_j$, the expenses of the mass of i th addition on the considered section of water object. In these designations the generalized model of transformation of i th addition on j th section of water object can be written down as follows:

$$C_{i,j+1}(n) = q_{i,j+1}(n)Q_{j+1}(n);$$
$$q_{i,j+1}(n) = F_{ij}(q_{ij}(n), q_{i1}(n),..., q_{ip}(n), \overline{\lambda_{ij}}, v_{ij}(n));$$
$$Q_{j+1}(n) = \psi_{ij}(Q_j(n), Q_1(n),..., Q_p(n), \overline{\lambda_{ij}}, v_{ij}(n)),$$

where $\overline{\lambda_{ij}} = (\lambda_{ij1},..., \lambda_{ijd})$ is d-dimension vector of unknown parameters; F_{ij}, ψ_{ij} are unknown functions.

The problem of statistical simulation consists in the selection of the structure of a model (form of functions F_{ij} and ψ_{ij}) and its unknown parameters by minimization of the chosen criterion:

$$\Phi(\widehat{F}_{ij}, \widehat{\psi}_{ij}, \widehat{\overline{\lambda}}_{ij}) = \sum_{n=1}^{N} \rho\left\{q_{ij}(n), Q_{j+1}(n), \widehat{F}_{ij}, \widehat{\psi}_{ij}, \widehat{\overline{\lambda}}_{ij}\right\} \cdot h(n) \to \min_{F,\psi\in\Omega,\bar{\lambda}_{ij}\in R^C},$$

where ρ is residual function; $h(n)$ is weight function, determining importance of information in n th moment of time; R^C is C-dimensional Euclidean space.

Depending on the selected form of functions F_{ij}, ψ_{ij} and residual function in works [1, 76-83] are offered statistical models of pollutants transport in the river. Some particular cases of functions F_{ij}, ψ_{ij} and critera of their identification are considered in the algorithms, given below in this chapter. Statistical models are widely applied in the problems of simulation of the state of water objects due to simplicity, stability to random fluctuations, absence of the requirements of deep analysis of passing physico-chemical processes.

For estimation of the quality of mathematical models, also their comparioson among themselves, there are necessary objective criteria of the effectiveness of these models. Such criteria are: accuracy of simulation, simplicity and visualization of developed models, requirements to the size and quality of necessary measurement information and so on. The most essential among them is the accuracy of simulation. The objective estimation of the accuracy of the developed models it is necessary to calculate of their quality by independent data which do not participate in the identification of models. In [76], as such criterion of effectiveness of models, is recommended the value $RR = S/\sigma^2$, where S is root-mean-square deviation of simulated process from the observed one; σ^2 is the variance of real

process. The value RR is the relative measure of the quality of mathematical model to the characteristic of dispersion of real process. It is proportional to the information quantity, obtained by model about real process. When the variance of real process is unknown and also its estimation is connected to certain difficulties, for comparison of qualities of two models, it is possible to use the criterion $R\widehat{R} = S_1 / S_2$, indicated the ratio between root-mean-square deviations of considered models [77].

Let us concider some, from huge number of existed works, devoted to the development of regression models.

In [51] are given the results of experimental comparison of accuracy of estimations of unknown parameters of the model by different methods. There are considered different regression models: classical regression, active regression experiments, passive observations. These methods are developed at fulfilment of the following suppositions: all variables have zero mean, the errors of independent variables do not correlate one another at different observations and have identical covariance matrix (in all observation points, errors of independent variables do not correlate with the error of dependent variable, errors of dependent variable do not correlate among themselves and their variance is equal to σ^2).

The problems of restoration of polynomial regression with exact values of independent variables at varying variance of dependent variable and with random values of independent variables at varying variance of dependent variable are considered in [52].

The robust algorithm for construction of point and interval estimations of the parameters of non-linear models, belonging to the class of internally linear models, i.e. non-linear models, which one by the help of transformation of the variables are reduced to the linear model, is given in [53]. The case of classic regression with constant variance of the dependent variable is considered.

The problem of obtaining robust estimations of coefficients of regression models is quite completely considered in [54, 55, 57]; the problem of restoration of linear regression at varying variance of dependent variable by the help of the method of weighed least squares is considered in [55]. In [57] is given a very wide range of statistical analysis methods - from exploratory analysis to causal inference to multi-level analysis. In particular, there also are described hierarchical models with a binary dependent variable.

In [56] is proposed an intelligent regression analysis methodology which is suitable for modeling massive datasets. The basic idea there is to split the entire dataset into several blocks, applying the classical regression techniques for data in each block, and finally combaining these regression results via weighted averages. Theoretical justification of the goodness of the proposed method and empirical performance based on extensive simulation study are given.

Steady autoregression models which are used for imitation of nonstationary, monotonically incrasing component in longitudinal data are given in [58].

General autoregression model has the following generalized form:

$$Y_i = X_i^* \theta + Z_i \xi_i + \varepsilon_i, \ \varepsilon_i \sim N_{n_i}(0, \sigma^2 I) \ \ (i = 1,..., N).$$

where

$$\varepsilon_{it} \sim N(0,\sigma^2),\ \ \theta_i = (\mu_i \phi_{i1} ... \phi_{ip} \beta_i^T) \sim N_{m+p+1}(\theta,\Omega),\ \ \theta = (\mu \phi_1 .. \phi_p \beta^T)^T,$$

$$X_{it}^* = (1 y_{i,t-1} ... y_{i,t-p} X_{it}^T)^T,\ \ X_i^* = (X_{i,p+1}^* ... X_{i,n_i}^*)^T,$$

$$\delta_i = (y_{i,1} ... y_{i,p})^T,\ \ Y_i = (y_{i,p+1} ... y_{i,n_i})^T,\ \ X_i = (X_{i,p+1} ... X_{i.n_i})^T,$$

$$Z_i = X_i^* Q,$$

$\{\varepsilon_{it}\}$ and $\{\theta_i\}$ are mutually independent and independent from $\{X_{it}\}$ variables. Formulae for calculation of the estimations of the parameters of the model in standard form and qualities of these estimations are given in [70].

In [59] is considered the following model

$$Y = \eta + \alpha,$$

$$(\eta, X_q) \sim N(1, \Sigma_{r+q}),\ \ \alpha \sim N(1, \phi),$$

where (η, X_q) and α are conditionally independent values with given covariance matrices Σ_{r+q} and ϕ of the sizes $(r+q)\times(r+q)$ and $r \times r$ respectively, i.e. $Y_{(1\times r)}$ is the sum of non observed value η and component of error α which are independent among themselves. Joint distribution η and independent variable $X_{q(1\times q)}$ is normal; α has independent normal distribution.

In the work is calculated

$$E(\eta^\ell \mid X_q^\ell, Y^\ell) = \omega_q Y^\ell + (1+\omega_q) X_q^\ell B_q^*,$$

where ω_q is some scalar value,

$$B_q^* = \{Q_{qq} + \omega_q (X_q^\ell)' X_q^\ell\}^{-1} \{Q_{q0} + \omega_q (X_q^\ell)' Y^\ell\},$$

where Q_{qq}, Q_{q0} are obtained by partition of positively defined matrix $Q_{r\times q}$ with sizes $(r+q)\times(r+q)$.

Bayes analysis for factor experiment is offered in [60]. There are given estimations of parameters and testing of hypothesis in a posterior analysis, using simple a priory conditions. Detailed formalization is realized for two factor models with replicae. Two illustrative applications on the basis of which author discuss realizability and representability of a posterior distributions, sensitivity and applicability of the methods of Monte Carlo for Markov chains are given.

Author of the work [61] uses Monte Carlo methods for discontinuous Markov chains [66] with the purpose of calculation of aposeriory distributions of hierarchical, graphical or decomposable log-linear models by high-dimensional tables of possible values. The choice of suitable prior distributions for the parameters of the model is also discussed in detail, and two examples are presented. The authors identify a lot of possible hierarchical, graphical and decomposable models and compare the obtained results with alternative approximations.

In [62] are given answers on the questions: does a regression model correspond to the true outlines? Do two regression models have the same outlines? How it is possible to group regression functions, based on outlines? These questions appear at investigating monotonicity, at calculation of local maximum or at studying variations in the family of curves. One can solve these questions by considering the rank correlation coefficient between two functions. This correlation is the generalisation of the rank correlation between two finite sets of numbers and is equal to one if and only if the two functions have the same outlines. The rank correlation based on smoothed estimates of regression functions in reality estimates true correlation. This rank correlation can be used as a measure of similarity of functions in cluster analysis and as a measure of monotonicity or modality.

The paper [63] propose a semiparametrical extension of the score method, offered in [67], for elimination of the shortage of the parameters. The procedure is developed for the cases when there are known the mean and the variance of the dependent variable and when average function contains both parameters: of benefity and of disparity. Important applications of semiparametric models include quasilikelihood models and models of error of the measurement [68]. The second important application is acceptance of the estimations for auxiliary functions [69] at solving simple linear systems which correspond to the true projection for the family canonical exponential distributions. Asymptotic properties and results of simulation show that the influance of peculiarities of the parameters is significantly reduced at using offered approach.

In [64] is realized theoretical research of two estimations of the parameters of partially linear model for grouped longitudinal data

$$Y_{ij} = X_{ij}^T \beta + \theta\left(T_{ij}\right) + \varepsilon_{ij},$$

where in i th group are contained m_i results of observation, β is vector with dimension $p \times 1$ and $\theta(\cdot)$ is unknown smooth function. Here ε_{ij} is the random error and, for different groups, they are independent. It is shown that for correlated data so called "basis proper" method [84] more often gives larger assimptotical divergence than "kernel profilated" method [85], i.e. estimations obtained by the second method are asymptotically more effective than the estimations obtained by the first method. The investigation of these methods is realized by imitative modeling of numerical experiments.

In [65] is considered the problem of obtaining, with the help of simple and generalized methods of least squares, estimations of the parameters of linear regression model

$$X_t = \mu + \alpha t + \varepsilon_t,$$

when errors $\{\varepsilon_t\}$ have zero means and are stationary in time with autocorrelations $\gamma(h)=\mathrm{cov}(\varepsilon_t,\varepsilon_{t+h})$ with the lag h. Correct expressions for estimating parameters of the regression are obtained for some time series with autocorrelation structure, including autoregression of the first order and generalized moving average. Application of the obtained results includes confidence intervals and example, in which the variance of estimation of the slope of the trend do not increase by increasing autocorrelation.

In [86] is considered self-renewing threshold autoregression model with changeable variance

$$x_t=\sum_{\ell=1}^{r+1}\left(b_0^{(\ell)}+\sum_{m=1}^{p_\ell}b_m^{(\ell)}x_{t-m}\right)I_{\left(\lambda_{\ell-1},\lambda_\ell\right)}\left(x_{t-d}\right)+\sigma\left(x_{t-1},...,x_{t-p}\right)\varepsilon_t,$$

where $\{\varepsilon_t\}$, $t=1,2,...,$ are independent identically distributed random variables with zero mean and unit variance, $\lambda_0=-\infty$ and $\lambda_{r+1}=\infty$. It is accepted that $p_\ell\le p$ for $\ell=1,2,...,r+1$, where p is known integral and $d\le p$, also $a<\lambda_1<\lambda_2<...<\lambda_r<b$, where a and b are two known constants.

Threshold autoregression models which are non linear models of time series, describing sudden changes in time, were considered in [87]. The most important parameters of these models are thresholds as they determine their nonlinear structures. Thresholds transform the models in different mode of operation, in each of which the structure of the model is linear. Hence, if thresholds are known, estimating other parameters, so as coefficients of regression, is relatively simple. However estimating thresholds is not simple task because, usualy, their number is not known and they are self-changeable points of the structure of the function. In [86] are considered the questions of estimating and testing of the thresholds in self-stimulating threshold autoregression models with unknown number of thresholds. There is offered statistical test, based on the empirical small wavy coefficients. There is given asymptotical distribution of statistical test and estimation of values of thresholds and their quantities. The Monte-Carlo method and real example, for teating realizability of the offered method, are used.

In the work [88] is considered partially linear model

$$\ln T_i=X_i\beta+h(R_i)+\varepsilon_i,$$

which contains non parametrical variable R - the period of diagnosis, for which is not defined more exactly the form of functional dependence for one or several compopnents. The mothod of identification of the regression, when dependent variable is censored, is offered in the work.

3.2. METHODS OF IDENTIFICATION OF NON-LINEAR REGRETIONS BY MODIFIED LEAST SQUARES CRITERION

General procedures of identification of non-linear regression relations is offered below, which one is developed with the purpose of overcoming two basic difficulties not only regression analysis but also all modern mathematics: non-linearity and multidimensionality of a problem [73-75]. The universal algorithm of optimum definition of regions of finding of unknown values of parameters of regression models, in which these unknown parameters with probability close to unit are contained, is developed. The quality of working and obtained results of iteration algorithms of search of extremum of criterion of identification depend on successful finding of these regions. Given methods is suitable for the rather wide class of non-linear regression models at classical regression and passive experiment and at its qualified application, in despite of usual non-linear estimation of parameters, considerably reduces the time necessary for solving identification problem and provides the given reliability. At some hardening of imposed restrictions on the nature of noises, the obtained results are also correct at active experiment.

The problem of identification of regression dependence is contained in the following. It is supposed that between observed variables x and y unknown functional dependence exists, which is approximated by the function of given class $f(a_1,...,a_m,x)$ on the basis of experimental data x_i, y_i, $i=1,..,N$, i.e. the truth of the following relation is supposed

$$y_i = f(a_1,...,a_m,x_i) + u_i,\ i=1,..,N, \tag{3.1}$$

where $a_1,...,a_m$ are unknowns coefficients, the values of which are estimated on the basis of observation results x_i, y_i, $i=1,..,N$; u_i are random fluctuations with the following characteristics $E(u_i)=0$, $V(u_i)=\sigma_i^2$, $\mathrm{cov}(u_i,u_j)=R_{ij}$, $i\neq j$, $i,j=1,...,N$.

The values of the parameters $a_1,...,a_m$ seek so that the weighed sum of the squared residuals

$$S=\sum_{i=1}^{N}\lambda_i\cdot\left|f(a_1,...,a_m,x_i)-y_i\right|^2 \tag{3.2}$$

would obtain minimum value; here λ_i are given weighted coefficients. The solution of this optimization problem determines statistical estimations $\hat{a}_1,...,\hat{a}_m$ of the suitable parameters (estimation of the method of least squares).

In case when restored relation is linear with respect to the parameters, searching their statistical estimations is not difficult: the problem is reduced to the solution of the system of m linear equations [89]. If the dependence of approximating function on the parameters is not linear, then for the solution of the considered problem there are used different iteration methods, including, when approximating function $f(a_1,...,a_m,x)$ is unsufficiently smooth

and its derivatives take large values in the domain of definition of parameters $a_1,...,a_m$, there are used iteration algorithms without using derivatives, including algorithm of Huk and Jivce [1, 90]. At application of these algorithms there are some difficulties, related to necessisity bound up with necessity of correct selection of the regions of seeking the parameters, since from it essentially depends the time of computation and reliability of obtained results.

The noted complexities of using iteration algorithms, at definition of a minimum of the functional (3.2), appear the more essential, than more is the number of parameters from which f function depends on non-linearly. A method is offered below, which one often allows to reduce the number of parameters, in relation to which the approximating function is non-linear.

Let us suppose that the sequence of unknown parameters of f function can be divided into two groups

$$[a_1,...,a_m]=[A_1,...,A_r,C_1,...,C_n]$$

($m=r+n$) so that the approximating function was linear with respect to the parameters $A_1,...,A_r$, i.e. the following representation is possible

$$f(a_1,...,a_m,x)=\sum_{k=1}^{r}A_k\cdot\varphi_k(C_1,...,C_n,x).$$

Then minimal value of (3.2), the sum of the squared residuals, at fixed values of $C_1,...,C_n$ is reached in a case, when the parameters $A_1,...,A_r$ satisfy the system of linear equations

$$\sum_{k=1}^{r}\alpha_{jk}A_k=B_j \qquad (j=1,...,r)$$

and it is equal to

$$S_\nu(C_1,...,C_n)=\sum_{L=1}^{N}\lambda_L\cdot y_L^2-\sum_{k=1}^{r}A_kB_k.$$

Here

$$\alpha_{jk}=\sum_{L=1}^{N}\lambda_L\cdot\varphi_j(C_1,...,C_n,x_L)\cdot\varphi_k(C_1,...,C_n,x_L);$$

$$B_j=\sum_{L=1}^{N}\lambda_L\cdot\varphi_j(C_1,...,C_n,x_L)\cdot y_L$$

are the coefficients dependent from $C_1,...,C_n$.

Estimations of the method of least squares of the parameters $C_1,...,C_n$ can be determined by different iteration methods, including the method of Huk and Jivce, in which the function $S_\nu(C_1,...,C_n)$ minimizes, and the estimations of the parameters $A_1,...,A_r$ find by solving the system of linear equations, and this system is necessary to solve at each next calculation of the function $S_\nu(C_1,...,C_n)$. The iteration process is stoped when the difference between neighbouring computed values of S_ν becomes less than a given value.

At rather general conditions, the least squares criterion, in which the functional (3.2) is minimized, can be changed by modified least squares criterion, in which is minimized the following quantity

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(g\left(f(a_1,...,a_m,x_i)\right) - g(y_i)\right)^2; \tag{3.3}$$

here g(y) is some suitable twice differentiable function; $\lambda' = \lambda_i / \left(\dot{g}(y_i)\right)^2$; $\dot{g}(y) = (d/dy)g(y).$

Considering (3.1), it is possible to rewrite (3.2) so

$$S = \sum_{i=1}^{N} \lambda_i \cdot u_i^2.$$

Using the formula of expansion of the function g (y) in the Taylor's series in the neighborhood of the points y_i and limiting by items of the order u_i^2, we shall obtain

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(g(y_i - u_i) - g(y_i)\right)^2 \approx$$

$$\approx \sum_{i=1}^{N} \lambda_i' \cdot \left(-\dot{g}(y_i) \cdot u_i + \frac{1}{2} \cdot \ddot{g}(y_i - v_i) \cdot u_i^2\right)^2 =$$

$$= \sum_{i=1}^{N} \lambda_i \cdot u_i^2 \cdot \left(1 - \frac{1}{2} \cdot \frac{\ddot{g}(y_i - v_i)}{\dot{g}(y_i)} \cdot u_i\right)^2,$$

where ν_i are the parameters, satisfying the conditions $0 < |\nu_i| < |u_i|$. Consequently, at

$$\left| \frac{\ddot{g}(y_i - v_i)}{\dot{g}(y_i)} \cdot u_i \right| < G$$

there takes place

$$S' = S \cdot (1 + \varepsilon / 2)^2, \tag{3.4}$$

where ε is the parameter satisfying the condition $|\varepsilon| \le G$.

The better the value S' approximates to S, the less is the value G, which one, from its side, depends on the character of the function g and the values of random components u_i. At given g and characteristics u_i always is possible to estimate maximum error of approximation (3.4) with given probability. The condition $G << 1$ is satisfyed, if the function $\dot{g}(y)$ is quite smooth and if residuals u_i are rather small. In many practical problems the latest condition happens executed.

The dependence of S'/S from standard deviations of residuals u_i, for different restoring dependences, is shown in Table 3.1; in each of four cases *a*)-*d*), the values of independent variable x_j are N equidistant points from the interval $[x_{\min}, x_{\max}]$; the residuals u_i are independent normally distributed random variables with zero mathematical expectations and variances σ^2; tables are composed for different values of $\sigma/(y_{\max} - y_{\min})$, where $y_{\max}$ and $y_{\min}$ are maximum and minimum values of the function $f(x_j)$, respectively. In the case *d*) we have $g(y) = 1/y$, in other cases - $g(y) = \ln y$.

In each concrete case the function $g(\cdot)$ is selected depending on approximating function $f(\cdot)$ so that as small as possible number of parameters, by which the functional S' is minimized, was non-linearly contained in it.

Finding estimations of the parameters, non-linearly contained in $g(\cdot)$, realizes by minimization of the functional S' by different iteration methods. For this methods is necessary to determine intervals, from domains of their definition, in which with unit probability are contained true values of the parameters.

Let us designate defined vector of non-linearly entering parameters by $c = (c_1, ..., c_n)$, and search regions of given parameter - by $[C_H, C_B]$. It is supposed that the given region is the hyperparallelepiped, bounded by coordinates of vectors C_H, C_B. For convergence of the algorithm, and also for minimization of necessary search time of estimations, the search region should be as small as possible; at this time, the probability of including true value of c in it should be close to unit.

One of universal, not dependent from a concrete kind of restored functional dependence, methods of definition of intervals of search of estimations of approximation parameters is offered below method, which is called *method of trials*. This method is universal and is applicable even when all parameters of the model are non-linearly included in it, i.e. when the estimations of the parameters are searched by direct minimization of the criterion (3.2).

The set of all points (x_j, y_j), $j = 1, ..., N$, of the plane (x, y), corresponding to the measured values, is divided into L groups, about n points in each group; here L is integer

part of the number N/n. For each of these groups, if it is possible, the interpolation of the function $f(c_1,...,c_n,x)$ realizes, i.e. such values of the parameters $c_1,...,c_n$ are determined, for which the graph of the function $f(c_1,...,c_n,x)$ passes through all n of points of the considered group. Let us call the sequence of *trial values* $\left[c^{(1)},c^{(2)},...,c^{(\nu)}\right]$ obtained by this way the sequence of the values of the parameter c; each trial value $c^{(k)}$ corresponds to one of groups of points (x_j,y_j), for which the interpolation of the function $f(c_1,...,c_n,x)$ is possible, i.e. the corresponding syatem of equations has the solution. The length of this sequence, evidently satisfy to the ratio $0 \le \nu \le L$. As bounds of search region C_H and C_B are taken vectors, the components of which are equal to minimum and maximum values of suitable components of the sequence of vectors $c^{(k)}$, $k = 1,...,\nu$.

Table 3.1.

a) $f(a,b,c,d,x) = a \cdot x^b \cdot e^{cx}$
$a = 6.240$; $b = 1.500$; $c = 1.300$;
$N = 100$; $x_{min} = 3.45$; $x_{max} = 4.0$;
$y_{min} = 3500$; $y_{max} = 9000$.

$\sigma/(y_{max}-y_{min})$	S_0	S'/S_0
0.10000	$9.203 \cdot 10^6$	1.07102
0.01000	92030.7	1.00715
0.00100	920.307	1.00072
0.00010	9.20307	1.00007

b) $f(a,b,c,d,x) = a \cdot x^b \cdot e^{cx}$
$a = 6.580$; $b = -5.000$; $c = 2.000$.
$N = 100$; $x_{min} = 1.15$; $x_{max} = 5.20$;
$y_{min} = 10.000$; $y_{max} = 56.87$.

$\sigma/(y_{max}-y_{min})$	S_0	S'/S_0
0.10000	667.514	1.21663
0.01000	6.67514	1.02213
0.00100	0.06675	1.00222
0.00010	0.00067	1.00022

c) $f(a,b,c,d,x) = a \cdot x^c \cdot (1-bx)^d$
$a = 4.500$; $b = 0.500$; $c = 2.300$; $d = 1.800$.
$N = 100$; $x_{min} = 0.620$; $x_{max} = 1.90$;
$y_{min} = 0.090$; $y_{max} = 1.332$.

$\sigma/(y_{max}-y_{min})$	S_0	S'/S_0
0.10000	0.46931	1.14703
0.01000	0.00469	1.01511
0.00100	0.00005	1.00151
0.00010	$4.69 \cdot 10^{-7}$	1.00015

d) $f(a,b,c,d,x) = 1/(a \cdot e^{cx} + b \cdot e^{dx})$
$a = 6.500$; $b = 2.300$;
$c = -1.000$; $d = 1.400$.
$N = 100$; $x_{min} = -0.75$; $x_{max} = 2.70$;
$y_{min} = 0.010$; $y_{max} = 0.120$.

$\sigma/(y_{max}-y_{min})$	S_0	S'/S_0
0.10000	0.00370	1.50605
0.01000	0.00004	1.04229
0.00100	$3.70 \cdot 10^{-7}$	1.00415
0.00010	$3.70 \cdot 10^{-9}$	1.00041

Described method of determination of the region $[C_H, C_B]$, to which should belong the parameter of approximation c, gives satisfactory result if the number of elements of the sequence of trial values of considered parameter $[c^{(1)}, c^{(2)}, ..., c^{(\nu)}]$ is quite big; otherwise, the given method requires some corrections. Let us call *modified trial method* described further method of definition of the region $[C_H, C_B]$.

Let us consider one dimensional case, i.e. when the function $f(\cdot)$ non-linearly contains only one parameter.

Let $C_{\min}$ and $C_{\max}$ are minimum and maximum trial values of the parameter c, respectively. The bounds of search interval are determined by the way

$$C_H = C_{\min} - h_\nu(\alpha) \cdot (C_{\max} - C_{\min});$$

$$C_B = C_{\max} + H_\nu(\alpha) \cdot (C_{\max} - C_{\min}), \tag{3.5}$$

where parameters $h = h_\nu(\alpha)$ and $H = H_\nu(\alpha)$ are determined as solutions of equations

$$\int_0^\infty \nu \cdot p(u) \cdot (\Phi(u) - \Phi(uh/(1+h)))^{\nu-1} du = \alpha/2;$$

$$\int_0^\infty \nu \cdot p(-u) \cdot (\Phi(-uH(1+H)) - \Phi(-u))^{\nu-1} du = \alpha/2; \tag{3.6}$$

$\Phi(c)$ and $p(c)$ are the function and the density of distribution of corresponding to c normalized random variable $(c - c^0)/\sigma$; $(1-\alpha)$ is probability that the true value of the parameter is contained in the interval $[C_H, C_B]$.

Theorem 3.1. *Let us suppose that the sequence of trial values* $[c^{(1)}, c^{(2)}, ..., c^{(\nu)}]$ *can be considered as sample corresponding to the determined on the interval* $(-\infty, +\infty)$ *random variable* c *with mathematical expectation* c^0. *Then determined by ratios (3.5), (3.6) interval is the confidence interval, to which belongs* c *with probability* $1-\alpha$.

The proof of the theorem is given in paragraph 3.5, where is considered the problem of finding consistent interval estimations for mathematical expectations of random variables with given probability distribution density. These results are used at determination of the initial interval of searching values of unknown parameters in the considered method of identification of non-linear regression.

In case when the distribution density of the random variable c is symmetrical, the equations (3.6) are equivalent, so that $h_\nu(\alpha) = H_\nu(\alpha)$. The values of coefficients

$h_\nu(\alpha) = H_\nu(\alpha)$ for different ν and α at normal probability distribution with arbitrary variance are viven in Table 3.2.

Table 3.2. The values of the coefficients $h_N(\alpha)$

α / N	0.1	0.05	0.02	0.01	0.005	0.002	0.001
2	2.6569	5.8531	15.410	31.328	63.161	158.65	317.81
3	0.3968	0.8133	1.6172	2.5129	3.7739	6.2700	9.0800
4	0.0538	0.2385	0.5409	0.8313	1.1926	1.8128	2.4225
5	–0.0784	0.0388	0.2133	0.3675	0.5467	0.8321	1.0934
6	–0.1485	–0.0612	0.0609	0.1627	0.2758	0.4473	0.5974
7	–0.1922	–0.1213	–0.0265	0.0493	0.1307	0.2498	0.3506
8	–0.2224	–0.1616	–0.0830	–0.0222	0.0413	0.1316	0.2061
9	–0.2445	–0.1906	–0.1227	–0.0715	–0.0191	0.0536	0.1122
10	–0.2616	–0.2126	–0.1521	–0.1075	–0.0626	–0.0016	0.0467
11	–0.2752	–0.2300	–0.1749	–0.1350	–0.0955	–0.0426	–0.0014
12	–0.2863	–0.2441	–0.1932	–0.1568	–0.1212	–0.0743	–0.0383
13	–0.2956	–0.2557	–0.2082	–0.1745	–0.1419	–0.0996	–0.0674
14	–0.3035	–0.2656	–0.2207	–0.1892	–0.1590	–0.1202	–0.0910
15	–0.3104	–0.2741	–0.2314	–0.2017	–0.1734	–0.1373	–0.1105
16	–0.3164	–0.2815	–0.2406	–0.2124	–0.1856	–0.1518	–0.1269
17	–0.3217	–0.2880	–0.2487	–0.2216	–0.1962	–0.1643	–0.1409
18	–0.3264	–0.2937	–0.2558	–0.2298	–0.2055	–0.1751	–0.1531
19	–0.3306	–0.2989	–0.2621	–0.2371	–0.2137	–0.1846	–0.1637
20	–0.3345	–0.3035	–0.2678	–0.2436	–0.2210	–0.1931	–0.1730
21	–0.3380	–0.3078	–0.2730	–0.2494	–0.2276	–0.2006	–0.1814
22	–0.3412	–0.3116	–0.2777	–0.2547	–0.2335	–0.2074	–0.1888
23	–0.3441	–0.3152	–0.2820	–0.2596	–0.2389	–0.2136	–0.1956
24	–0.3468	–0.3184	–0.2859	–0.2640	–0.2438	–0.2192	–0.2017
25	–0.3493	–0.3214	–0.2895	–0.2681	–0.2483	–0.2243	–0.2073
26	–0.3516	–0.3242	–0.2929	–0.2718	–0.2525	–0.2290	–0.2125
27	–0.3538	–0.3268	–0.2960	–0.2753	–0.2564	–0.2334	–0.2172
28	–0.3559	–0.3293	–0.2989	–0.2786	–0.2600	–0.2374	–0.2216
29	–0.3578	–0.3316	–0.3017	–0.2817	–0.2633	–0.2412	–0.2256
30	–0.3596	–0.3337	–0.3042	–0.2845	–0.2665	–0.2447	–0.2294
40	–0.3732	–0.3499	–0.3234	–0.3057	–0.2897	–0.2704	–0.2570
50	–0.3821	–0.3603	–0.3356	–0.3192	–0.3043	–0.2864	–0.2740
60	–0.3884	–0.3678	–0.3444	–0.3288	–0.3146	–0.2976	–0.2859
70	–0.3933	–0.3735	–0.3510	–0.3360	–0.3224	–0.3061	–0.2948
80	–0.3971	–0.3781	–0.3563	–0.3418	–0.3286	–0.3127	–0.3018
90	–0.4003	–0.3818	–0.3606	–0.3465	–0.3336	–0.3182	–0.3075
100	–0.4030	–0.3849	–0.3643	–0.3504	–0.3379	–0.3228	–0.3123
200	–0.4176	–0.4020	–0.3839	–0.3718	–0.3607	–0.3473	–0.3379
300	–0.4243	–0.4097	–0.3929	–0.3815	–0.3710	–0.3584	–0.3495

At fixed α with increase of sample size ν the function $h_\nu(\alpha)$ decreases and, as from some value of ν, namely - at $\nu > \log_2(2/\alpha)$, it becomes negative. This means that the interval $[C_H, C_B]$, determined by modified trial method, does not extend the interval

$[C_{\min}, C_{\max}]$ but narrows down it. At $\nu \to \infty$, $h_\nu(\alpha) \to -1/2$. This means that the interval $[C_H, C_B]$ at $\nu \to \infty$ degenerates in point, located in the middle of the interval $[C_{\min}, C_{\max}]$.

From Table 3.2 it is evident that to determine search region of the parameters, non-linearly included in approximating function, is possible even at $\nu = 2$, but increasing ν narrows down search region and, by that, reduces the time necessary for working iteration algorithms of search of estimations of the parameters and increases reliability of obtained reasults. It is obvious that, the less is the search region, the less is the probability that except of a global minimum in it is contained local minima of the functional S.

Let us consider the problem of distribution of trial values of parameters of the identification. Let values of regression variable are equal to $y_i = Y_i + u_i$ $(i = 1,...,N)$, where Y_i are the exact values of restored function in the points x_i; u_i are independent normally distributed residuals with mathematical expectations equal to zero and variances σ_i^2.

Each set of trial values $c_1^{(j)},...,c_n^{(j)}$, is the solution of the system of equations

$$f\left(c_1^{(j)},...,c_n^{(j)}, x_{J_r}\right) = Y_{J_r} + u_{J_r}; \quad J_r \in (1,...,N), \quad r = 1,...,n, \quad J_1 \neq J_2 \neq ... \neq J_n,$$

which in general form can be written down as

$$c_r^{(j)} = f_r^{-1}\left(y_{J_1},...,y_{Jn}, x_{J_1},...,x_{Jn}\right); \quad r = 1,...,n. \tag{3.7}$$

If in right sides of these ratios to substitute $u_{J_1} = ... = u_{Jn} = 0,$ trial values $c_1^{(j)},...,c_n^{(j)}$ will coincide with exact values $c_1^0,...,c_n^0$ of the suitable parameters. Let us decompose the functions f_r^{-1}, $r = 1,...,n$, in neighborhoods of Y_{J_r}, $r = 1,...,n$, in the Taylor's series and satisfy by items of the first order. We shall obtain

$$c_r^{(j)} \approx c_r^o + \mu_{r1} u_{J_1} + ... + \mu_{rm} u_{Jn}; \quad r = 1,...,n, \tag{3.8}$$

where μ_{pr} are elements of the matrix, inverse to $[T_{pr}]$, and

$$T_{pr} = \frac{\partial}{\partial c_r^{(j)}} f(c_1^{(j)},...,c_n^{(j)}, x_{J_p}); \quad p,r = 1,...,n.$$

If (x_{J_r}, y_{J_r}) select so that they are on quasilinear parts of the function f_r^{-1}, $r = 1,...,n$, then the errors of approximation (3.8) is so minimal that in practical computations they can be neglected. The following fact is obvious, the rule of selection of points (x_{J_r}, y_{J_r}), $r = 1,...,n$, depends on concrete kinds of the function (3.7) and varys from a problem to other problem.

Hence, if the linear approximation of the dependence of $c_r^{(j)}$ from residuals is permissible, then c is normally distributed random vector with mathematical expectation c^0 and covariance matrix $[W_{jk}]$, where

$$W_{jk} = \sum_{L=1}^{n} \mu_{jL}\mu_{kL}\sigma_{J_L}^2, \qquad j,r = 1,...,n.$$

The statistical distributions of parameters c differ from normal when their dependences (3.7) from interpolation points essentially differ from linear. The degree of non-linearity of these dependences is determined by non-linear items in the Taylor series, where the basic contribution in non-linearity bring in quadratic items

$$\sum_{i=1}^{n}\sum_{k=1}^{n} \chi_{ik}^{(r)} u_{J_i} u_{J_k},$$

where

$$\chi_{ik}^{(r)} = \frac{\partial^2 c_r}{\partial Y_{J_i}\partial Y_{J_k}} = -\sum_{s=1}^{n}\sum_{p=1}^{n}\sum_{q=1}^{n} \mu_{rs}\cdot \vartheta_{pq}^{(s)} \cdot \mu_{pi}\mu_{qk};$$

$$\vartheta_{pq}^{(s)} = \frac{\partial^2 f\left(c_1^{(j)},...,c_n^{(j)}, x_{J_s}\right)}{\partial c_p^{(j)}\partial c_q^{(j)}} \qquad (r,i,k,s,p,q = 1,...,n).$$

Hence, for maximum approaching the distribution of the parameter c_r to normal, it is necessary to select the points (x_{J_r}, y_{J_r}), $r = 1,...,n$, so that the norm of the matrix $[\chi_{jk}^{(r)}]$ was minimal.

At correctness of the approximation (3.8), the probabilities of falling the vector c in the hyperparallelepiped with borders $[C_H^i, C_B^i]$, $i = 1,...,n$, is equal to

$$I = \int_{C_H}^{C_B} (2\pi)^{-n/2} \,|\det W|^{-1/2} \cdot \exp\left(-\frac{1}{2} X^T W^{-1} X\right) dX. \qquad (3.9)$$

If for each component of the vector c we take the confidence probability close to unit, then, naturally, the probability (3.9), of falling the vector c in the confidence hyperparallelepiped, is close to unit too. At construction of the confidence hyperparallelepiped, with guaranteed value of the confidence probability, it is necessary to act as follows: to expand independently computed borders of confidence intervals for each component of the vector c so that there take place $I = 1-\alpha$. For computation of multidimensional integral (3.9) it is possible to use the modified method of Monte-Carlo [1, 91].

Some examples, illustrated the essence described modified method of trials are given below. The algorithms of identification of some noon-linear functional dependences and the results of investigation of their basic properties are given in Appendix 4 [106]. These algorithms are developed on the basis of offered in this paragraph modified method of trials.

In summary we will consider one more modification of described above methods of determination of boundaries of parametres of approximation based on use of splines.

In the trial method and the modified trial method the auxiliary problem of interpolation of the restored dependence is used. While, as it is shown below (see Section 3.4), this problem often is considerably simplified in the case of equidistant values of argument; it takes place for many concrete types of restored dependence containing limited quantity of parameters.

In such cases it is possible to offer the following method of determination of boundaries: if there are given N values of the investigated function y_j in points x_j, not being equidistant from each other ($j = 1,..,N$), then

- for determination of approximate values of the investigated function in additional points the cubic spline $s(x)$ corresponding to available pairs of points $[x_j, y_j]$ ($j = 1,..,N$), is used;
- in the least interval containing all points x_j, N equidistant from each other values of the argument x'_1, x'_2, ..., x'_N are determined and approximate values of the investigated function in these points y'_1, y'_2, ..., y'_N; $y'_j = s(x'_j)$ are considered ($j = 1,..,N$);
- boundaries of search of approximation parameters are determined by the the modified trial method for N pairs of points $[x'_j, y'_j]$ ($j = 1,..,N$).

Examples

For illustration of modified trial method, as examples, we shall consider the following functional dependences: a) $f(a,b,c,x) = a + b \cdot e^{c \cdot x}$; b) $f(a,b,c,d,x) = a \cdot e^{c \cdot x} + b \cdot e^{d \cdot x}$; c) $f(h,a,b,c,d,x) = h + a \cdot e^{c \cdot x} + b \cdot e^{d \cdot x}$. The values of the number ν and borders of the intervals of searching of the parameters of approximation are given in Table 3.3. They are obtained by unmodified and modified trial methods. The restored function depends on non-linearly from these parameters. In each of three cases a)-c), the values of independent variable x_j are N equidistant points from the interval $[x_{\min}, x_{\max}]$; residuals u_j are independent normally distributed random variables with mathematical expectations equal to zero and variances σ^2. The tables are composed for different values of $\sigma/(y_{\max} - y_{\min})$, where $y_{\max}$ and $y_{\min}$ are maximum and minimum values of the function $f(x_j)$, respectively.

From obtained results is evident that in determined intervals of the search of true values of the parameters of the regression in reality are contained these values and the intervals are narrowed down at decreasing the mean square deviation of observation results of dependent variable of the regression.

Table 3.3.

a) $f(a,b,c,x) = a + b \cdot e^{cx}$

$N = 100$; $x_{min} = -0.050$; $x_{max} = 2.500$; $y_{min} = 7.516$; $y_{max} = 238.5$;

$a = 6.500$; $b = 2.500$; $c = 1.800$.

$\sigma/(y_{max}-y_{min})$	ν	$[c_{min}, c_{max}]$	$[c_H, c_B]$
0.10000	29	[–0.249; 4.479]	[1.244; 2.987]
0.01000	33	[1.541; 2.029]	[1.699; 1.871]
0.00100	33	[1.772; 1.821]	[1.788; 1.805]
0.00010	33	[1.797; 1.802]	[1.799; 1.800]

b) $f(a,b,c,d,x) = a \cdot e^{cx} + b \cdot e^{dx}$

$N = 100$; $x_{min} = -2.000$; $x_{max} = 2.000$; $y_{min} = -39.75$; $y_{max} = 40.05$;

$a = -5.400$; $b = 2.480$; $c = -1.000$; $d = 1.400$.

σ/(ψμαξ–ψμιν)	ν	[χμιν, χμαξ]	[χH, χB]	[δμιν, δμαξ]	[δH, δB]
0.1000	23	[–3.599; 0.069]	[–2.507;–1.022]	[0.013; 2.452]	[0.739; 1.727]
0.0100	25	[–1.113;–0.934]	[–1.058;–0.989]	[1.221; 1.494]	[1.304; 1.411]
0.0010	25	[–1.011;–0.994]	[–1.006;–0.999]	[1.381; 1.409]	[1.390; 1.401]
0.0001	25	[–1.001;–0.999]	[–1.001;–1.000]	[1.398; 1.401]	[1.399; 1.400]

c) $f(h,a,b,c,d,x) = h + a \cdot e^{cx} + b \cdot e^{dx}$

$N = 100$; $x_{min} = -2.000$; $x_{max} = 2.000$; $y_{min} = -18.75$; $y_{max} = 61.05$;

$h = 21.00$; $a = -5.400$; $b = 2.480$; $c = -1.000$; $d = 1.400$.

σ/(ψμαξ–ψμιν)	ν	[χμιν, χμαξ]	[χH, χB]	[δμιν, δμαξ]	[δH, δB]
0.1000	9	[–4.409;–0.195]	[–3.754;–0.851]	[0.726; 4.610]	[1.330; 4.006]
0.0100	20	[–1.486;–0.668]	[–1.253;–0.901]	[0.883; 1.758]	[1.132; 1.509]
0.0010	20	[–1.045;–0.964]	[–1.022;–0.987]	[1.338; 1.429]	[1.364; 1.403]
0.0001	20	[–1.004;–0.996]	[–1.002;–0.999]	[1.394; 1.403]	[1.396; 1.400]

At restoration of considered functional dependences, the sampl, composed by trial values of searching parameters, is possible to use for testing the hypothesis of normality of distribution of these values. Let, analogously of the above, the values of independent variable are given in equidistant points from the interval $[x_{\min}, x_{\max}]$. In Figure 3.1 a) and b) are given the graphs of trial values c_j (on the axis of abscissa is arranged the number j) for restored dependences $a + b \cdot e^{c \cdot x}$ and $a \cdot e^{c \cdot x} + b \cdot e^{d \cdot x}$, respectively. In the first case are used the following initial data: $a = 6.5$; $b = 2.5$; $c = 1.8$; $x_{\min} = -0.5$; $x_{\max} = 2.5$; $N = 760$; $\sigma/(y_{\max} - y_{\min}) = 0.1$; at the same time, the number of trial values is equal to $\nu = 154$; in the second case, the initial datas are the following: $a = 6.5$; $b = 2.3$; $c = -1$; $d = 1.4$; $x_{\min} = -2.5$; $x_{\max} = 2.5$; $N = 760$; $\sigma/(y_{\max} - y_{\min}) = 0.1$; at the same time, the number of trial values is equal to $\nu = 92$.

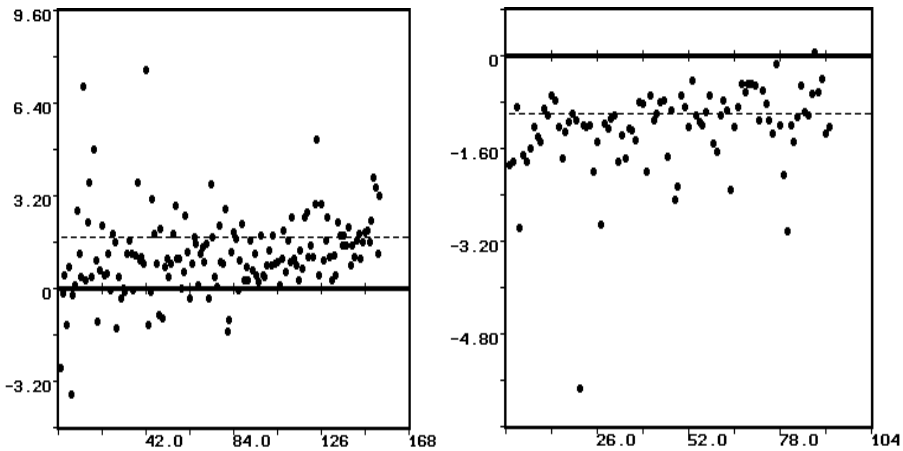


Figure 3.1. The graphs of trial values of the parameter c.

In Figure 3.2 a) and b) are presented the histograms corresponding to given sampls. In both cases, testing normality of the distribution of trial values of c, by criterions of the chi-square, the Kolmogorov-Smirnov and the Omega-square, gives positive results. In particular, in the criterion of chi-square, for the first sampl, the value of statistics $\chi^2 = 17.487$, and percentage points, determining acceptance region of the hypothesis with significance level 0.95, are equal to $\chi^2_{\alpha/2} = 3.2227$ and $\chi^2_{1-\alpha/2} = 20.481$, respectively; for the second sampl these values are equal to $\chi^2 = 13.343$, $\chi^2_{\alpha/2} = 1.6899$ and $\chi^2_{1-\alpha/2} = 16.013$, respectively.

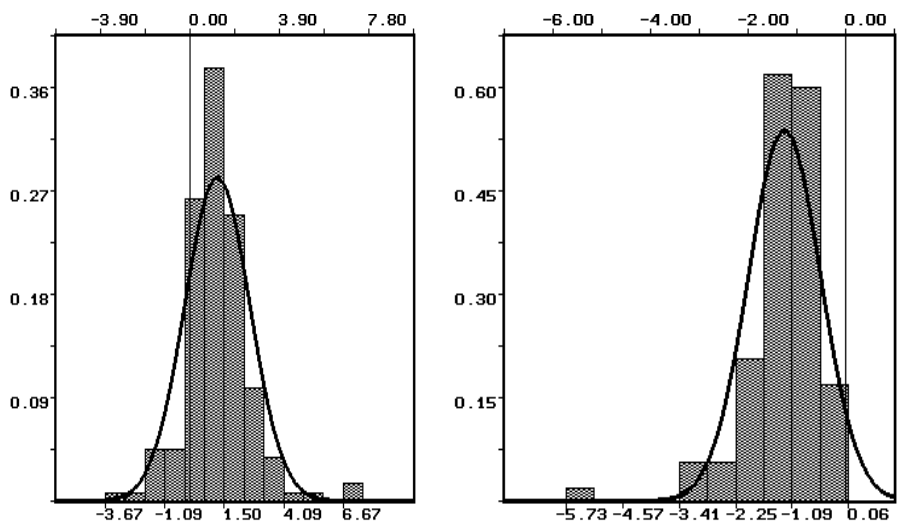


Figure 3.2. Probability distribution densities of trial values of the parameter c.

The offered above methodology of identification of nonlinear regressions are widely used in developed by authors application package of processing experimental information for IBM-compatible computers [92-94, 101, 226], in section "Identification of functional dependences". The application of this package at solving many practical problems from different domains of knowledge, including modeling pollution of rivers, was demonstrated the universality, the regularity and the reliability of the methodology [1, 74, 95-100].

3.3. RESTORATION OF POLYNOMIAL REGRESSION ON THE BASIS OF ACTIVE EXPERIMENT

The algorithm of restoration of polynomial regression at varying variances both dependent and independent variables is offered below [1, 44]. Optimum properties of the offered algorithm are demonstrated experimentally. The polynomial regression finds broad application at restoration of functional dependences between observed quantities. Moreover, in considerable part of measurement devices, the restoration of calibration curves are realized on the basis of active experiment (for example, graduation of spectrometers of the energy of gamma-quantums, graduation of the spectrometer for the measurement of nuclear emission with inductively related plasma etc. [53]).

Development of the algorithm. Polynomial regression at activ experiment looks like

$$y_i = \sum_{j=1}^{m+1} a_j x_i^{j-1} + \varepsilon_i, \quad x_i = x_{0i} + \delta_i, \quad i = 1,...,N, \tag{3.10}$$

where x_{0i} is true value of independent variable, at which the researcher observs dependent variable y_i, but because of random noises δ_i, imposed on x_{0i} to the value y_i corresponds random variable x_i; δ_i and ε_i are random fluctuations, for which there take place

$$\begin{aligned} &E(\delta_i) = E(\varepsilon_i) = 0, \quad V(\delta_i) = \sigma_{x_i}^2, \quad V(\varepsilon_i) = \sigma_{\varepsilon_i}^2, \\ &\operatorname{cov}(\delta_i, \delta_j) = \operatorname{cov}(\delta_i, \varepsilon_j) = \operatorname{cov}(\varepsilon_i, \varepsilon_j) = 0, \quad i \neq j; \end{aligned} \tag{3.11}$$

$a_1,...,a_{m+1}$ are unknowns coefficients of the regression, the values of which is necessary to estimate on the basis of y_i and x_{0i}, $i = 1,...,N$.

Let us rewrite (3.10) as follows:

$$y = \sum_{j=1}^{m+1} a_j (x_{0i} + \delta_i)^{j-1} + \varepsilon_i = \sum_{j=1}^{m+1} a_j x_{0i}^{j-1} + \sum_{j=2}^{m+1} a_j \left(\sum_{\ell=1}^{j-1} C_\ell^{j-1} x_{0i}^{j-\ell-1} \delta_i^\ell \right) + \varepsilon_i,$$

where C_ℓ^{j-1} is the number of combinations ℓ from $j-1$. Let us designate

$$\gamma_i = \sum_{j=2}^{m+1} a_j \left(\sum_{\ell=1}^{j-1} C_\ell^{j-1} x_{0i}^{j-\ell-1} \delta_i^\ell \right) + \varepsilon_i.$$

Then (3.10) will take the form

$$y_i = \sum_{j=1}^{m+1} a_j x_{0i}^{j-1} + \gamma_i, i = 1,..., N. \tag{3.12}$$

Accordingly

$$E(\gamma_i) = \sum_{j=2}^{m+1} a_j \left[\sum_{\ell=1}^{j-1} C_\ell^{j-1} x_{0i}^{j-\ell-1} E(\delta_i^\ell) \right]; \tag{3.13}$$

$$E(\gamma_i^2) = \sum_{j=2}^{m+1} \sum_{p=2}^{m+1} a_j a_p \left[\sum_{\ell=1}^{j-1} \sum_{t=1}^{p-1} C_\ell^{j-1} \; C_t^{p-1} \; x_{0i}^{j+p-\ell-t-2} \; E(\delta_i^{\ell+t}) \right] + \sigma_{\varepsilon_i}^2; \tag{3.14}$$

$$\operatorname{cov}(\gamma_i, \gamma_k) = 0, \quad i \neq k;$$

$$V(\gamma_i) = \sum_{j=2}^{m+1} \sum_{p=2}^{m+1} a_j a_p \left\{ \sum_{\ell=1}^{j-1} \sum_{t=1}^{p-1} C_\ell^{j-1} C_t^{p-1} x_{0i}^{j+p-\ell-t-2} \times \left[E(\delta_i^{\ell+t}) - E(\delta_i^\ell) E(\delta_i^t) \right] \right\} + \sigma_{\varepsilon_i}^2. \tag{3.15}$$

The form of the formula for calculation of $E(\delta_i^\ell)$ depends on probability distribution function of the random variable δ_i. In accordance with [102], at $\delta_i \sim N(\cdot;0,\sigma_{x_i}^2)$, there takes place

$$E(\delta_i^\ell) = \begin{cases} 0 \;\; at \;\; odd \;\; \ell, \\ \dfrac{\ell!}{2^{\ell/2}(\ell/2)!} \sigma_{x_i}^\ell \;\; at \;\; even \;\; \ell. \end{cases}$$

Thus, the active experiment (3.19) can be presented as passive experiment (3.12), where $E(\gamma_i)$ and $V(\gamma_i)$ are determined by formulae (3.13) and (3.15), respectively, and $\operatorname{cov}(\gamma_i, \gamma_j) = 0$ at $i \neq j$.

For finding unknown coefficients $a_1,...,a_{m+1}$, let us use the method of weighed least squares

$$S = \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{m+1} a_j x_{0i}^{j-1} \right)^2 \lambda_i \Rightarrow \min_{\{a_j\}}. \tag{3.16}$$

Let us designate

$$A^T = (a_1, a_2, ..., a_{m+1}); \quad Y_\lambda^T = (\sqrt{\lambda_1} y_1, ..., \sqrt{\lambda_N} y_N);$$

$$X_\lambda^0 = \begin{pmatrix} \sqrt{\lambda_1}, & \sqrt{\lambda_2} & \dots & \sqrt{\lambda_N} \\ \sqrt{\lambda_1} x_{01}, & \sqrt{\lambda_2} x_{02} & \dots & \sqrt{\lambda_N} x_{0N} \\ \dots & \dots & \dots & \dots \\ \sqrt{\lambda_1} x_{01}^m, & \sqrt{\lambda_2} x_{02}^m & \dots & \sqrt{\lambda_N} x_{0N}^m \end{pmatrix}.$$

In those designations, the system of normal equations, obtained from (3.16), will be written down as

$$X_\lambda^0 Y_\lambda = X_\lambda^0 X_\lambda^{0T} A.$$

from here

$$A = \left(X_\lambda^0 X_\lambda^{0T} \right)^{-1} X_\lambda^0 Y_\lambda. \tag{3.17}$$

Let us calculate mathematical expectation and variance of the estimation (3.17). Let us designate $\nu_\lambda^T = (\sqrt{\lambda_1}\nu_1, ..., \sqrt{\lambda_N}\nu_N)$. Then $Y_\lambda = X_\lambda^{0T} A^0 + \nu_\lambda$, where A^0 is the vector of true values of desired coefficients. From the ratio (3.17), we obtain

$$E(A) = A^0 + (X_\lambda^0 X_\lambda^{0T})^{-1} X_\lambda E(\nu_\lambda); \tag{3.18}$$

$$V(A) = (X_\lambda^0 X_\lambda^{0T})^{-1} X_\lambda^0 E(\nu_\lambda \nu_\lambda^T) X_\lambda^{0T} (X_\lambda^0 X_\lambda^{0T})^{-1}.$$

Let us calculate elements of the matrix $E(\nu_\lambda \nu_\lambda^T)$. Let us designate $V_\lambda = \nu_\lambda \nu_\lambda^T$, i.e. $v_{ij}^\lambda = \sqrt{\lambda_i \lambda_j}\nu_i \nu_j$. Then

$$\begin{aligned} &E\left(v_{ij}^\lambda\right) = \sqrt{\lambda_i \lambda_j} \cdot E\left(\gamma_i\right) \cdot E\left(\gamma_j\right) \quad at \quad i \neq j; \\ &E\left(v_{ii}^\lambda\right) = \lambda_i \cdot E\left(\gamma_i^2\right) \quad at \quad i = j. \end{aligned} \tag{3.19}$$

where $E(\nu_i)$ and $E(\nu_i^2)$ are determined in accordance with formulae (3.13) and (3.14).

Estimations of the coefficients $a_1,...,a_{m+1}$, calculated by the ratio (3.17), are biased. It is not difficult to obtain unbiased estimations

$$A_{несм} = A - \left(X_\lambda^0 X_\lambda^{0T}\right)^{-1} X_\lambda^0 E\left(\gamma_\lambda\right). \tag{3.20}$$

Let us choose weight coefficients λ_i, $i=1,...,N$, so that the variance of the estimation of the coefficients A, calculated by formulae (3.18), (3.19), was minimum. For this purpose, let us determine λ_i as follows: $\lambda_i = \left[E\left(\gamma_i^2\right)\right]^{-1}$. In that case, it is not difficult to be convinced that $E\left(v_{ij}^\lambda\right) < 1$ at $i \neq j$ and $E\left(v_{ii}^\lambda\right) = 1$ at $i = j$.

The calibration points $x_{0i}, i = 1,...,N$, are chosen so that the variance of the estimation of unknown coefficients $V(A)$ was minimum. On the other hand, for simplification of identification problem, it is necessary to strive to the decrease of the number of calibration points. In accordance with [102], for determination of the polynomial of m order, no more than $m+1$ of different values of x is necessary, from which no more than $m-1$ of the values should be inside the interval. Thus, it is possible to suppose that $N = m+1$. Then, it is possible to rewrite (3.18) as:

$$V(A) = \left(X_\lambda^{0T}\right)^{-1} E\left(\gamma_\lambda \gamma_\lambda^T\right) X_\lambda^{0-1}. \tag{3.21}$$

Let us consider the problem of choice of $m-1$ internal points from the interval of definition of the regression $\left(x_0^{'}, x_0^{''}\right)$ for minimization of spread matrix (3.21) of estimations of the parameters. With regard to (3.19), the minimum of the variance (3.21) is reached by maximization of elements of the matrix X_λ^0. By direct maximization of elements of the matrix X_λ^0 on the interval $x \in [-1;+1]$, we are convinced that optimal values of calibration points $x_{02},...,x_{0m}$, for the interval $[-1;+1]$, are:

Degree of the polynomial	Values of calibration points from $[-1;+1]$
1	± 1;
2	± 1; 0
3	± 1; $\pm 0{,}4472$
4	± 1; $\pm 0{,}6547$; 0
5	± 1; $\pm 0{,}7651$; $\pm 0{,}2852$
6	± 1; $\pm 0{,}8302$; $\pm 0{,}4689$; 0

At $N = m+1$, formulae (3.17), (3.20) take the forms

$$A = \left(X_{\lambda}^{0T}\right)^{-1} Y_{\lambda}; \tag{3.22}$$

$$A_{несм} = \left(X_{\lambda}^{0T}\right)^{-1} \left(Y_{\lambda} - E\left(\gamma_{\lambda}\right)\right). \tag{3.23}$$

Estimations, calculated by ratio (3.20) or (3.23), are unbiased and inconsistent. For obtaining consistent estimations, instead of the model of observation (3.10), it is necessary to use the following model:

$$y_{ip} = \sum_{j=1}^{m+1} a_j x_{ip}^{j-1} + \varepsilon_{ip}, \quad p = 1,..., n_i; \tag{3.24}$$

$$x_{ip} = x_{0i} + \delta_{ip}, \quad i = 1,..., N;$$

$$E(\delta_{ip}) = E(\varepsilon_{ip}) = 0, \quad V(\delta_{ip}) = \sigma_{x_i}^2, \quad V(\varepsilon_{ip}) = \sigma_{\varepsilon_i}^2,$$

$$\operatorname{cov}(\delta_{ip}, \delta_{jt}) = \operatorname{cov}(\delta_{ip}, \varepsilon_{jt}) = \operatorname{cov}(\varepsilon_{ip}, \varepsilon_{jt}) = 0.$$

Let us rewrite (3.24) as follows:

$$y_{ip} = \sum_{j=1}^{m+1} a_j x_{0i}^{j-1} + \sum_{j=2}^{m+1} a_j \left(\sum_{l=1}^{j-1} C_{\ell}^{j-1} x_{0i}^{j-\ell-1} \delta_{ip}^{\ell} \right) + \varepsilon_{ip}, \tag{3.25}$$

$$p = 1,..., n_i; \quad i = 1,..., N.$$

Let us average the results of observation for each value of independent variable

$$y_i = \frac{1}{h_i} \sum_{p=1}^{h_i} y_{ip} = \sum_{j=1}^{m+1} a_j x_{0i}^{j-1} + \sum_{j=2}^{m+1} a_j \left(\sum_{\ell=1}^{j-1} C_{\ell}^{j-1} x_{0i}^{j-\ell-1} \frac{1}{h_i} \sum_{p=1}^{h_i} \delta_{ip}^{\ell} \right) + \frac{1}{h_i} \sum_{p=1}^{h_i} \varepsilon_{ip}. \tag{3.26}$$

Let us designate

$$\frac{1}{h_i} \sum_{p=1}^{h_i} \delta_{ip}^{\ell} = \delta_i^{\ell}; \quad \frac{1}{h_i} \sum_{p=1}^{h_i} \varepsilon_{ip}. = \varepsilon_i.$$

At this time

$$E(\delta_i) = E(\varepsilon_i) = 0, \quad V(\delta_i) = \sigma_{x_i}^2 / n_i, \quad V(\varepsilon_i) = \sigma_{\varepsilon_i}^2 / n_i,$$

$$\operatorname{cov}(\delta_i, \delta_j) = \operatorname{cov}(\delta_i, \varepsilon_j) = \operatorname{cov}(\varepsilon_i, \varepsilon_j) = 0, \quad i \neq j;$$

In introduced designations, the model (3.26) transforms to the model (3.10). All obtained results remain valid. Estimations of unknown coefficients, in this case, will be consistents, as at $n_i \to \infty$, $i = 1,..., N$, the variance of the vector of estimations of unknown coefficients

(3.21) tends to zero. Really, at $n_i \to \infty$, there takes place $E\left(\gamma_i^2\right) \to 0$, $E\left(\gamma_\lambda \gamma_\lambda^T\right)$ does not change, and elements of the matrix X_λ^0 tend to the infinity.

In accordance with [44, 103], α percentage joint confidence interval, for true values of coefficients of considered regression, looks like

$$P\left[\left(A^0 - A_{несм}\right)^T V^{-1}\left(A\right)\left(A^0 - A_{несм}\right) \le \frac{m+1}{1-\alpha}\right] \ge \alpha.$$

Unfortunately, direct use of the algorithm (3.23), for calculation of estimations of coefficients of polynomial regression, is impossible, as the same coefficients are included in it. Therefore, the search of the coefficients is realized in two steps. On the first step, estimations of the coefficients are calculated by the formula (3.22), at supposition that x_i are nonrandom values. Weigh coefficients are determined as follows $\lambda_i = \left(\sigma_{\varepsilon_i}^2\right)^{-1}$. On the second step, by the help of estimations of unknown coefficients, obtained on the first step by the formula (3.23), in which the suitable weights are determined by the ratio (3.21), approximations of unknown coefficients are iteratively calculated until the norm of the difference between vectors of coefficients of neighboring approachs will not be less than a given value.

For illustration of properties of the algorithm (3.23) and its advantages by comparison with the algorithm (3.22), below are given the results of experimental investigation of these algorithms for concrete regression dependence $y = 1 + 1.5x + 2x^2$. In Figure 3.3-3.6 are shown dependences of variances D_1 and D_2 of restored regressions, calculated by formulae (3.22) and (3.23). The following characteristics of the regression are accepted: $m = 2;$ $N = 3;$ $x \in [1;5];$ $x_{01} = 1;$ $x_{02} = 3;$ $x_{03} = 5;$ $n_1 = n_2 = n_3 = 10;$ $\sigma_{x_1}^2 = 0.1;$ $\sigma_{x_2}^2 = 0.2;$ $\sigma_{x_3}^2 = 0.3;$ $\sigma_{\varepsilon_1}^2 = 1;$ $\sigma_{\varepsilon_2}^2 = 1.5;$ $\sigma_{\varepsilon_3}^2 = 2$. Reduced in Figure 3.3-3.6 dependences confirm the fact that the varience of restored regression decreases at increasing the number of observations in calibration points and it increases at increasing the variances both dependent and independent variables.

Non monotonicity of the suitable dependences from the number of repeated observations for dependent variable (see Figure 3.3) are determined by randomness of obtained estimations. From Figure 3.6, it is seen that for each concrete regression there is optimum length of the region of its definition. Curves in Figure 3.5 confirm reduced above results about optimum choice of values of independent variable. From dependences, the fact of advantage of the algorithm (3.23) by comparison with the algorithm (3.22), is obvious. The results of operation of the algorithm (3.22) are designated by D_1 and ΔA_1, and the algorithm (3.23) - by D_2 and ΔA_2.

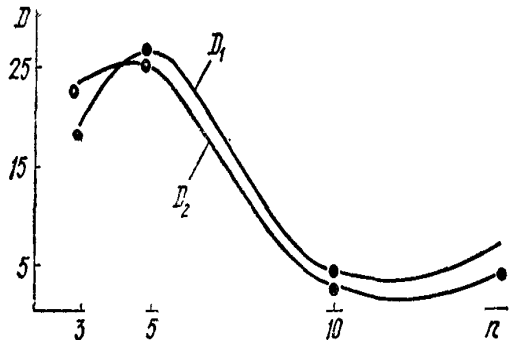


Figure 3.3. Dependence of the variance of restored regression from the number of repeated observations) of dependent variable.

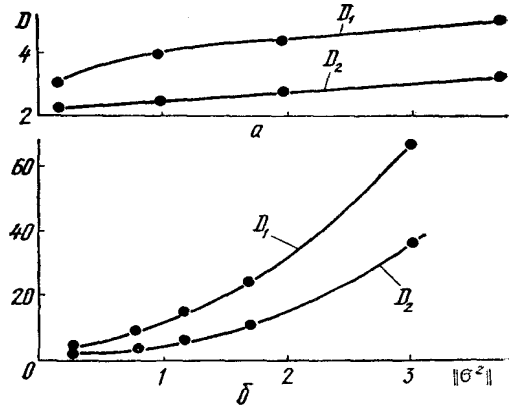
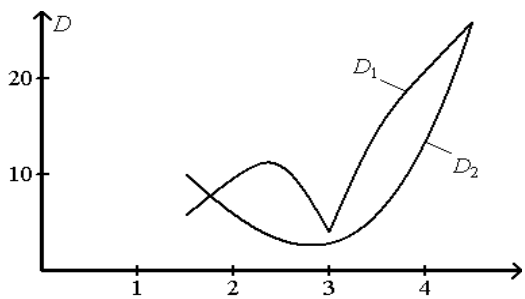
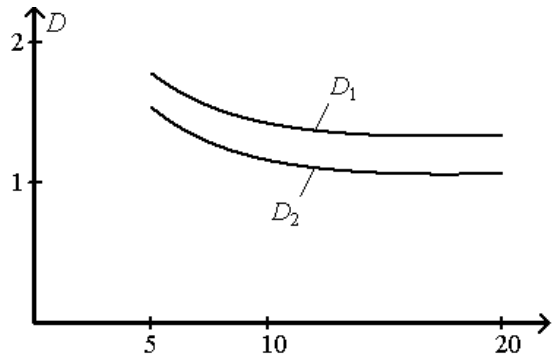


Figure 3.4. Dependence of the variance of restored regression from the variance of defendent (a) and independent (b) variables.



Position of the midpoint of the interval of definition of regression.

Figure 3.5. Dependence of the variance of restored regression from the choice of the values of independent variable in the interval of definition of the regression.



Length of the interval of definition of the regression.

Figure 3.6. Dependence of the norm of deviation of estimations of parameters from the length of the interval of definition of the parameters.

3.4. INTERPOLATION OF NONLINEAR FUNCTIONS OF CERTAIN CLASS

The problem of interpolation of nonlinear functions arises at solving many different problems of sciences and practice. For example, at restoration of nonlinear functional dependences by the data, do not cantaned random errors; at solving approximation problems by methods of spline-analysis (see paragraph 1.4); at determination of initial intervals of domain of parameters in problems of identification of nonlinear regressions (see paragraph 3.2) [1, 108] etc. Therefore, the development of optimum algorithms of interpolation of nonlinear functional dependences and their investigation are actual problems, having wide practical application.

Algorithms of interpolation of one-parameter families of functions from polynomials and some nonlinear functions are given below. These functions are very often used at restoration of functional dependnces in many practical applications. These algorithms are used by authors in developed by them universal program package of processing experimental information for PC-compatible personal computers in section of restoration of functional dependences for finding optimum initial intervals of definition of unknown parameters of these dependences [1, 93, 94, 110] and at solving many practical problems concerning to the identification of regression models of pollutants transport in the rivers.

3.4.1. One-parametrical Families of Functions of Polynomials

Let $[z_0, z_1, ..., z_N]$ and $[w_0, w_1, ..., w_N]$ be sequences of complex numbers; $z_j \neq z_k$ at $j \neq k$, $j,k = 0,1,...,N$; $\psi(\gamma, z, w)$ is complex function of three variables. It is required to determine the polynomial of the power $N-1$

$$\alpha(z)=\sum_{k=0}^{N-1}\alpha_k.z^k$$

and numeric parameter γ, for which the values of the function $\psi(\gamma,z,\alpha(z))$ in given nodal points $z_0,z_1,...,z_N$ coincide with numbers $w_0,w_1,...,w_N$, respectively.

Let us introduce auxiliary functions

$$\rho^{(m)}(\xi_1,\xi_2,...,\xi_m) \text{ and } \lambda_{jk}^{(m)}(\xi_1,\xi_2,...,\xi_m)$$

($m=1,2,...,j$, $k=1,2,...,m$), determined for the sequence m complex numbers $\xi_1,\xi_2,...,\xi_m$ as follows: values $\lambda_{jk}^{(m)}(\xi_1,\xi_2,...,\xi_m)$ are elements of the matrix, inverse to quadratic matrix

$$\mu^{(m)}=\begin{bmatrix} 1, & \xi_1, & \xi_1^2, & ..., & \xi_1^{m-1} \\ 1, & \xi_2, & \xi_2^2, & ..., & \xi_2^{m-1} \\ ... & ... & ... & ... & ... \\ 1, & \xi_m, & \xi_m^2, & ..., & \xi_m^{m-1} \end{bmatrix}$$

of m order, and

$$\rho^{(m)}(\xi_1,\xi_2,...,\xi_m)\equiv\det\left(\mu^{(m)}\right)=\prod_{k=2}^{m}\prod_{j=1}^{k-1}(\xi_k-\xi_j)$$

is the determinant of the Vandermonde for numbers $\xi_1,\xi_2,...,\xi_m$ [109].

Theorem 3.2. *If at any fixed values γ and z the function $\Psi(\xi)=\psi(\gamma,z,w)$ has inverse function $\Phi(\eta)=\varphi(\gamma,z,\eta)$, then parameters $\alpha_0,\alpha_1,...,\alpha_{N-1}$ can be determined by the parameter γ and initial data of the problem by the ratios*

$$\alpha_{k-1}=\sum_{j=1}^{N}\lambda_{kj}^{(N)}(z_1,z_2,...,z_N)\cdot\varphi(\gamma,z_j,w_j), \tag{3.27}$$

and the parameter γ is the solution of the equation

$$\sum_{k=0}^{N}\beta_k\cdot\varphi(\gamma,z_k,w_k)=0, \tag{3.28}$$

where

$$\beta_k = (-1)^k \cdot \rho^{(N)}(z_0,..., z_{k-1}, z_{k+1},..., z_N)\,.$$

In particular, at $N = 2$

$$\beta_0 = z_2 - z_1; \quad \beta_1 = z_0 - z_2; \quad \beta_2 = z_1 - z_0\,;$$

at $N = 3$

$$\beta_0 = (z_3 - z_1)(z_3 - z_2)(z_2 - z_1); \quad \beta_1 = -(z_3 - z_2)(z_3 - z_0)(z_2 - z_0);$$
$$\beta_2 = (z_3 - z_1)(z_3 - z_0)(z_1 - z_0); \quad \beta_3 = -(z_2 - z_1)(z_2 - z_0)(z_1 - z_0).$$

Proof. Let's consider the system of equations

$$\alpha(z_k) = \varphi(\gamma, z_k, w_k) \quad (k = 0,1,2,..., N),, \tag{3.29}$$

At the fixed value γ.

For justification of Formula (3.27) it is enough to notice that the system of equations (3.29) at $k = 1,..., N$ represents conditions of interpolation for the polynomial assuming given values in given points. According to conditions of the problem determinant of the given system of equations is nonzero, whence univalentity of its solution follows.

For derivation of formulas (3.28) let's remark that system (3.29) represents the system of $N+1$ linear equations with N unknowns α_0, ..., α_{N-1}; in order to this system have solution it is necessary that determinant of the matrix

$$\begin{bmatrix} 1, & z_0, & z_0^2, & ..., & z_0^{N-1} & \varphi(\gamma, z_0, w_0) \\ 1, & z_1, & z_1^2, & ..., & z_1^{N-1} & \varphi(\gamma, z_1, w_1) \\ ... & ... & ... & ... & ... & ... \\ 1, & z_N, & z_N^2, & ..., & z_N^{N-1} & \varphi(\gamma, z_N, w_N) \end{bmatrix}$$

is equal to zero. Expanding this determinant by elements of the last column we will obtain necessary result.

Examples:

a) At interpolation of logarithmic-polynomial dependence

$$\psi\big(\gamma, z, \alpha(z)\big) = \gamma \cdot \ln\left(\sum_{k=0}^{N} \alpha_k\, z^k\right),$$

the parameter γ can be determined as solution of the equation

$$\sum_{k=0}^{N} \beta_k \, e^{w_k / \gamma} = 0,$$

and coefficients of the polynomial are equal to

$$\alpha_{k-1} = \sum_{j=1}^{N} \lambda_{kj}^{(N)}(z_1, z_2, ..., z_N) \cdot e^{w_j / \gamma}, \qquad k = 1, ..., N .$$

b) At interpolation of geometric-polynomial dependence

$$\psi\left(\gamma, z, \alpha(z)\right) = z^{\gamma} \cdot \sum_{k=0}^{N} \alpha_k \, z^k$$

also exponential-polynomial dependence

$$\psi\left(\gamma, z, \alpha(z)\right) = e^{\gamma z} \cdot \sum_{k=0}^{N} \alpha_k \, z^k ,$$

the parameter γ and coefficients of the polynomial are determined by ratios

$$\sum_{k=0}^{N} \beta_k \, w_k \cdot z_k^{-\gamma} = 0 ;$$

$$\alpha_{k-1} = \sum_{j=1}^{N} \lambda_{kj}^{(N)}(z_1, z_2, ..., z_N) \cdot w_j \cdot z_j^{-\gamma}, \qquad k = 1, ..., N ,$$

or, accordingly,

$$\sum_{k=0}^{N} \beta_k \, w_k \cdot e^{-\gamma z_k} = 0 ;$$

$$\alpha_{k-1} = \sum_{j=1}^{N} \lambda_{kj}^{(N)}(z_1, z_2, ..., z_N) \cdot w_j \cdot e^{-\gamma z_j}, \qquad k = 1, ..., N .$$

3.4.2. Nonlinear Functions of the Certain Class of Limited Quantity of Parameters

1. Function $a+b\cdot e^{cx}$

Let be necessary to interpolate the function $a+b\cdot e^{cx}$ using three paired numbers $\{x_1,y_1\}$, $\{x_2,y_2\}$, $\{x_3,y_3\}$; otherwise, it is required to solve the system of equations

$$a+b\cdot e^{cx_1}=y_1;\quad a+b\cdot e^{cx_2}=y_2;\qquad a+b\cdot e^{cx_3}=y_3$$

with respect to parameters a,b,c. The conditions $x_1\neq x_2\neq x_3$ and $y_1\neq y_2\neq y_3$ are supposed executed. Let us introduce auxiliary quantity

$$s=\frac{y_3-y_2}{y_2-y_1};\ \text{then}\ s+1=\frac{y_3-y_1}{y_2-y_1}.$$

The parameter c is a nonzero solution of the equation

$$(y_2-y_3)\cdot e^{cx_1}+(y_3-y_1)\cdot e^{cx_2}+(y_1-y_2)\cdot e^{cx_3}=0.$$

The parameters a and b are determined by ratios

$$a=\frac{y_2\cdot e^{cx_1}-y_1\cdot e^{cx_2}}{e^{cx_1}-e^{cx_2}}=\frac{y_3\cdot e^{cx_2}-y_2\cdot e^{cx_3}}{e^{cx_2}-e^{cx_3}};$$
$$b=\frac{y_1-y_2}{e^{cx_1}-e^{cx_2}}=\frac{y_2-y_3}{e^{cx_2}-e^{cx_3}}.$$

If values of the argument are equidistant from each other, i.e. $x_2-x_1=x_3-x_2\equiv\Delta x$, then the initial system of equations has the solution in and only in the following case, if $s>0$; at this case $c=\ln S/\Delta x$.

Let $x_1<x_2<x_3$. The initial system of equations has the solution in and only in the case, if $s>0$. The equation, which must be satisfied by the parameter c, is convenient be presented as $f(c)=0$, where

$$f(c)=s-(s+1)\cdot e^{(x_2-x_1)\cdot c}+e^{(x_3-x_1)\cdot c}.$$

The graph of the function $f(c)$ to within parallel carry looks like introduced in Figure 3.7. The number

$$c_0 = (x_3 - x_2)^{-1} \cdot \ln\left((s+1) \cdot \frac{x_2 - x_1}{x_3 - x_1} \right)$$

is the point of minimum of the function $f(c)$; the number

$$c_1 = (x_3 - x_2)^{-1} \cdot \ln\left((s+1) \cdot \left(\frac{x_2 - x_1}{x_3 - x_1} \right)^2 \right)$$

is the abscissa of the point of inflection of the graph of the function $f(c)$; the number

$$c_2 = (x_3 - x_2)^{-1} \cdot \ln(s+1)$$

is the upper bound of c.

As an initial approach for c at solving the equation $f(c) = 0$ by iterative method of Newton, there can be taken the number c_1 (at $c_0 < 0$) or c_2 (at $c_0 > 0$).

Let us note also that $c / c_0 > 1$.

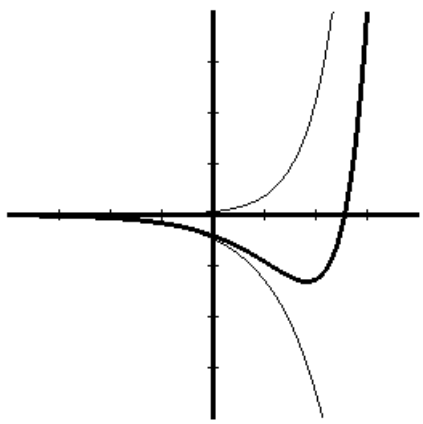


Figure 3.7.

2. Function $(a + bx) \cdot e^{cx}$

Let be necessary to interpolate the function $(a + bx) \cdot e^{cx}$ using three paired numbers $\{x_1, y_1\}$, $\{x_2, y_2\}$, $\{x_3, y_3\}$, i.e. to solve the system of equations

$$(a + b\,x_1) \cdot e^{cx_1} = y_1; \quad (a + b\,x_2) \cdot e^{cx_2} = y_2; \quad (a + b\,x_2) \cdot e^{cx_3} = y_3$$

with respect to parameters a, b, c.

The parameter c is the root of the equation

$$(x_2 - x_3)\cdot y_1 \cdot e^{-cx_1} + (x_3 - x_1)\cdot y_2 \cdot e^{-cx_2} + (x_1 - x_2)\cdot y_3 \cdot e^{-cx_3} = 0.$$

The parameters a and b are determined by ratios

$$a = \frac{1}{x_2 - x_1}\cdot (x_2 \cdot y_1 \cdot e^{-cx_1} - x_1 \cdot y_2 \cdot e^{-cx_2});$$
$$b = \frac{1}{x_2 - x_1}\cdot (-y_1 \cdot e^{-cx_1} + y_2 \cdot e^{-cx_2}).$$

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 \equiv \Delta x$, then the value $u \equiv \exp(c\cdot \Delta x)$ satisfy to the quadratic equation

$$y_1 \cdot u^2 - 2y_2 \cdot u + y_3 = 0.$$

Let $x_1 < x_2 < x_3$. The equation, which must be satisfied by the parameter c, is convenient to be presented as $f(c) = 0$, where

$$f(c) = H_1 \cdot e^{(x_3 - x_1)c} + H_2 \cdot e^{(x_3 - x_2)c} + H_3;$$
$$H_1 = y_1 \cdot (x_2 - x_3); \quad H_2 = y_2 \cdot (x_3 - x_1); \quad H_3 = y_3 \cdot (x_1 - x_2).$$

Depending on signs of numbers y_1, y_2 and y_3, several cases are possible:

a) $y_1 \cdot y_2 \le 0$ and $y_2 \cdot y_3 \le 0$. The function $f(c)$ has no zeros.

b) $y_1 \cdot y_2 \le 0$ and $y_2 \cdot y_3 > 0$. The function $f(c)$ has unique zero, as an initial approach for which, at solving the equation $f(c) = 0$ by iterative method of Newton, can be taken the number

$$\max\left\{\frac{1}{x_3 - x_2}\cdot \ln\left(\frac{-H_3}{H_1 + H_2}\right), \frac{1}{x_3 - x_1}\cdot \ln\left(\frac{-H_3}{H_1 + H_2}\right)\right\}$$

(being upper bound of c).

c) $y_1 \cdot y_2 > 0$ and $y_2 \cdot y_3 < 0$. The function $f(c)$ has unique zero, as an initial approach for which, at solving the equation $f(c) = 0$ by iterative method of Newton, can be taken the number

$$\max\left\{\frac{1}{x_2-x_1}\cdot\ln\left(\frac{H_2+H_3}{-H_1}\right),\ \frac{1}{x_3-x_1}\cdot\ln\left(\frac{H_2+H_3}{-H_1}\right)\right\}$$

(being upper bound of c).

d) $y_1\cdot y_2>0$ and $y_2\cdot y_3>0$. Let us introduce supplementary designations:

$$c_0=(x_2-x_1)^{-1}\cdot\ln(y_2/y_1);\qquad \Delta c=(x_2-x_1)^{-1}\cdot\ln\left(\frac{x_3-x_2}{x_3-x_1}\right);$$

$$v_0=\left(\frac{-H_3}{f(c_0)-H_3}\right)^{x_2-x_1}=y_1^{x_3-x_2}\cdot y_2^{x_1-x_3}\cdot y_3^{x_2-x_1}=(y_3/y_2)^{x_2-x_1}\cdot(y_1/y_2)^{x_3-x_2}.$$

(c_0 is the point of extremum of the function $f(c)$; $c_0-\Delta c$ is the abscissa of the point of inflection of the given function).

At $v_0<0$ the function $f(c)$ has two zeros c' and c''. Let us suppose for definiteness $c'<c''$; then $c'<c_0<c''<c_0+\Delta c$. The numbers $c_0-\Delta c$ and $c_0+\Delta c$ can be used as initial approachs for c' and c'', respectively, at solving the equation $f(c)=0$ by iterative method of Newton.

At $v_0=1$, the function $f(c)$ has one zero, coinciding with c_0.

At $v_0>1$, the function $f(c)$ have no zeros.

3. Function $h+(a+bx)\cdot e^{cx}$

Let be necessary to interpolate the function $h+(a+bx)\cdot e^{cx}$ using four paired numbers $\{x_1,y_1\}$, $\{x_2,y_2\}$, $\{x_3,y_3\}$, $\{x_4,y_4\}$, i.e. to solve the system of equations

$$h+(a+bx_1)\cdot e^{cx_1}=y_1;\ h+(a+bx_2)\cdot e^{cx_2}=y_2;\ h+(a+bx_3)\cdot e^{cx_3}=y_3;$$
$$h+(a+bx_4)\cdot e^{cx_4}=y_4$$

with respect to parameters h,a,b,c.

Parameter c is a nonzero solution of the equation $f(c)=0$, where

$$f(c)=(y_3-y_4)\cdot(x_2-x_1)\cdot e^{c\cdot(x_1+x_2)}+(y_2-y_4)\cdot(x_1-x_3)\cdot e^{c\cdot(x_1+x_3)}+$$
$$(y_2-y_3)\cdot(x_4-x_1)\cdot e^{c\cdot(x_1+x_4)}+(y_1-y_4)\cdot(x_3-x_2)\cdot e^{c\cdot(x_2+x_3)}+$$
$$(y_1-y_3)\cdot(x_2-x_4)\cdot e^{c\cdot(x_2+x_4)}+(y_1-y_2)\cdot(x_4-x_3)\cdot e^{c\cdot(x_3+x_4)}.$$

The number 0 always is zero point of functions $f(c)$ and $f'(c)$.

Parameters h, a and b are determined by ratios

$$a = \frac{1}{D}\left(y_1 \cdot (x_2 \cdot e^{cx_2} - x_3 \cdot e^{cx_3}) + y_2 \cdot (x_3 \cdot e^{cx_3} - x_1 \cdot e^{cx_1}) + y_3 \cdot (x_1 \cdot e^{cx_1} - x_2 \cdot e^{cx_2})\right),$$

$$b = \frac{-1}{D}\left(y_1 \cdot (e^{cx_2} - e^{cx_3}) + y_2 \cdot (e^{cx_3} - e^{cx_1}) + y_3 \cdot (e^{cx_1} - e^{cx_2})\right),$$

$$h = \frac{1}{D}\left(y_1 \cdot (x_3 - x_2) \cdot e^{c(x_2+x_3)} + y_2 \cdot (x_1 - x_3) \cdot e^{c(x_3+x_1)} + y_3 \cdot (x_2 - x_1) \cdot e^{c(x_1+x_2)}\right),$$

where

$$D = (x_3 - x_2) \cdot e^{c(x_2+x_3)} + (x_1 - x_3) \cdot e^{c(x_3+x_1)} + (x_2 - x_1) \cdot e^{c(x_1+x_2)}).$$

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 \equiv \Delta x$, then the value $u \equiv \exp(c \cdot \Delta x)$ satisfys to the quadratic equation

$$(y_2 - y_1) \cdot u^2 + 2(y_2 - y_3) \cdot u + (y_4 - y_3) = 0.$$

Let us suppose that the quotients of differences between any set values of the argument are equal to some rational numbers. Then values of the argument can be presenteded as $x_k = X_c + r_k \cdot \Delta x,$ where $r_k (k = 1,2,3)$ are some integers; $X_c, \Delta x = const$. In this case, the value $u \equiv \exp(c \cdot \Delta x)$ is the root of algebraic equation

$$r_{43} \cdot (y_2 - y_1) \cdot u^{r_{21}+2r_{32}+r_{43}} + 2 \cdot (r_{32} + r_{43}) \cdot (y_1 - y_3) \cdot u^{r_{21}+r_{32}+r_{43}} +$$
$$+ r_{32} \cdot (y_4 - y_1) \cdot u^{r_{21}+r_{32}} + (r_{21} + r_{32} + r_{43}) \cdot (y_3 - y_2) \cdot u^{r_{32}+r_{43}} +$$
$$+ (r_{21} + r_{32}) \cdot (y_2 - y_4) \cdot u^{r_{32}} + r_{21} \cdot (y_4 - y_3) = 0,$$

where $r_{jk} \equiv r_j - r_k$; $j, k = 1,2,3$.

4. Function $a \cdot x^c \cdot (1 - bx)^d$

Let be necessary to interpolate the function $a \cdot x^c \cdot (1 - bx)^d$ using four paired numbers $\{x_1, y_1\}$, $\{x_2, y_2\}$, $\{x_3, y_3\}$, $\{x_4, y_4\}$, i.e. to solve the system of equations

$$a x_1^c \cdot (1 - bx_1)^d = y_1; \quad a x_2^c \cdot (1 - bx_2)^d = y_2; \quad a x_3^c \cdot (1 - bx_3)^d = y_3; \quad a x_4^c \cdot (1 - bx_4)^d = y_4$$

with respect to parameters a, b, c, d. Let us designate

$Z_k \equiv \ln x_k, \quad W_k \equiv \ln y_k, \quad k = 1,2,3,4.$

The parameter b is a nonzero solution of the equation $f(b) = 0$, where

$$f(b) = H_1 \cdot \ln(1 - b \cdot x_1) + H_2 \cdot \ln(1 - b \cdot x_2) + H_3 \cdot \ln(1 - b \cdot x_3) + H_4 \cdot \ln(1 - b \cdot x_4);$$
$$H_1 = W_2 \cdot (Z_4 - Z_3) + W_3 \cdot (Z_2 - Z_4) + W_4 \cdot (Z_3 - Z_2);$$
$$H_2 = W_1 \cdot (Z_3 - Z_4) + W_3 \cdot (Z_4 - Z_1) + W_4 \cdot (Z_1 - Z_3);$$
$$H_3 = W_1 \cdot (Z_4 - Z_2) + W_2 \cdot (Z_1 - Z_4) + W_4 \cdot (Z_2 - Z_1);$$
$$H_4 = W_1 \cdot (Z_2 - Z_3) + W_2 \cdot (Z_3 - Z_1) + W_3 \cdot (Z_1 - Z_2).$$

The number 0 always is zero point of the function $f(b)$.

Let's assume that $x_1 < x_2 < x_3 < x_4$, and we will consider the equation $f(b) = 0$. This equation can have only unique real nonzero solution.

For existence of such solution, it is necessary that the quadratic equation

$$p_2 \, u^2 + p_1 \, u + p_0 = 0,$$

where

$$p_0 = -(H_1 \, x_1 + H_2 \, x_2 + H_3 \, x_3 + H_4 \, x_4);$$
$$p_1 = (H_1 + H_2) \, x_1 x_2 + (H_1 + H_3) \, x_1 x_3 + (H_1 + H_4) \, x_1 x_4$$
$$+ (H_2 + H_3) \, x_2 x_3 + (H_2 + H_4) \, x_2 x_4 + (H_3 + H_4) \, x_3 x_4;$$
$$p_2 = -\big((H_1 + H_2 + H_3) \, x_1 x_2 x_3 + (H_1 + H_2 + H_4) \, x_1 x_2 x_4$$
$$+ (H_1 + H_3 + H_4) \, x_1 x_3 x_4 + (H_2 + H_3 + H_4) \, x_2 x_3 x_4\big),$$

had two real roots.

Let u_1 and u_2 are the real roots of this equation, and $u_1 < u_2$. Then if $u_1 < 0 \;\; u_2 > 0$ and $H_4 \, f(u_2) > 0$ then the equation $f(b) = 0$ has a positive root contained in the interval $(u_2, 1/x_4)$;

if $u_1 < 0$, $u_2 < 0$ and $f(u_1) f(u_2) < 0$ then the equation $f(b) = 0$ has a negative root contained in the interval (u_1, u_2);

in other cases the equation $f(b) = 0$ has no nonzero real roots.

Proof:

The coefficients appearing in the expression for $f(b)$ satisfy to the relations

$$\sum_{k=1}^{4} H_k = 0 \text{ and } \sum_{k=1}^{4} H_k \ln H_k = 0.$$

It follows from here that this function at $b < 0$ can be presented in the form

$$f(b) = \sum_{k=1}^{4} H_k \cdot \ln(1 - b\, x_k) = \sum_{k=1}^{4} H_k \cdot \ln\left(1 - 1/(b\, x_k)\right).$$

Natural domain of definition of the function $f(b)$ is the open interval $(-\infty, 1/x_4)$; at approach to boundaries of this interval it takes place

$$\lim_{b \to -\infty} f(b) = 0 \quad \text{and} \quad \lim_{b \to 1/x_4} f(b) = (-\operatorname{sign} H_4) \cdot \infty.$$

Points of extremum of the function $f(b)$ if they are available coincide with roots of the quadratic equation $p_2\, u^2 + p_1\, u + p_0 = 0$. If this equation has no real roots then the function $f(b)$ everywhere is monotone and, hence, its unique zero is the point $b = 0$.

If u_1 and u_2 $(u_1 \le u_2)$ are points of extremum of the function $f(b)$ then each of the intervals $(-\infty, u_1)$, (u_1, u_2), $(u_2, +\infty)$ can contain no more than one zero of the function $f(b)$ since in these intervals the function $f(b)$ is monotone. But in the interval $(-\infty, u_1)$ the function $f(b)$ does not become zero owing to that it monotonically tends to zero at $b \to -\infty$. There remain two intervals (u_1, u_2) and $(u_2, +\infty)$, one of which contains solution of the equation $f(b) = 0$ equal to zero, and the second one can contain nonzero solution of this equation if only on the boundaries of this interval the function $f(b)$ has different signs.

Further all is obvious.

After that the parameter b is determined, the parameters a, c and d are determined by relations

$$\ln a = T^{-1} \cdot (W_2 Z_3 - W_3 Z_2) \cdot \ln(1 - b x_1) + T^{-1} \cdot (W_3 Z_1 - W_1 Z_3) \cdot \ln(1 - b x_2) + \\ + T^{-1} \cdot (W_1 Z_2 - W_2 Z_1) \cdot \ln(1 - b x_3);$$

$$c = T^{-1} \cdot (W_3 - W_2) \cdot \ln(1 - b x_1) + T^{-1} \cdot (W_1 - W_3) \cdot \ln(1 - b x_2) + \\ + T^{-1} \cdot (W_2 - W_1) \cdot \ln(1 - b x_3);$$

$$d = T^{-1} \cdot (W_1 (Z_3 - Z_2) + W_2 (Z_1 - Z_3) + W_3 (Z_2 - Z_1)),$$

where

$$T = (Z_3 - Z_2)\cdot\ln(1 - bx_1) + (Z_1 - Z_3)\cdot\ln(1 - bx_2) + (Z_2 - Z_1)\cdot\ln(1 - bx_3).$$

5. Function $a\cdot e^{cx} + b\cdot e^{dx}$

Let be necessary to interpolate the function $a\cdot e^{cx} + b\cdot e^{dx}$ using four paired numbers $\{x_1, y_1\}$, $\{x_2, y_2\}$, $\{x_3, y_3\}$, $\{x_4, y_4\}$, i.e. to solve the system of equations

$$a\,e^{cx_1} + b\,e^{dx_1} = y_1;\quad a\,e^{cx_2} + b\,e^{dx_2} = y_2;\quad a\,e^{cx_3} + b\,e^{dx_3} = y_3;\quad a\,e^{cx_4} + b\,e^{dx_4} = y_4$$

with respect to parameters a, b, c, d.

The pair of numbers $[c, d]$ can be determined as the solution of any pair of the following four equations

$$\begin{aligned}
&y_1\cdot(e^{cx_2+dx_3} - e^{cx_3+dx_2}) + y_2\cdot(e^{cx_3+dx_1} - e^{cx_1+dx_3}) + y_3\cdot(e^{cx_1+dx_2} - e^{cx_2+dx_1}) = 0;\\
&y_2\cdot(e^{cx_3+dx_4} - e^{cx_4+dx_3}) + y_3\cdot(e^{cx_4+dx_2} - e^{cx_2+dx_4}) + y_4\cdot(e^{cx_2+dx_3} - e^{cx_3+dx_2}) = 0;\\
&y_1\cdot(e^{cx_2+dx_4} - e^{cx_4+dx_2}) + y_2\cdot(e^{cx_4+dx_1} - e^{cx_1+dx_4}) + y_4\cdot(e^{cx_1+dx_2} - e^{cx_2+dx_1}) = 0;\\
&y_1\cdot(e^{cx_3+dx_4} - e^{cx_4+dx_3}) + y_3\cdot(e^{cx_4+dx_1} - e^{cx_1+dx_4}) + y_4\cdot(e^{cx_1+dx_3} - e^{cx_3+dx_1}) = 0
\end{aligned}$$

at additional condition $c \neq d$.

Parameters a and b are determined by ratios

$$a = \frac{y_1\cdot e^{dx_4} - y_4\cdot e^{dx_1}}{e^{cx_1+dx_4} - e^{cx_4+dx_1}};\qquad b = \frac{-y_1\cdot e^{cx_4} + y_4\cdot e^{cx_1}}{e^{cx_1+dx_4} - e^{cx_4+dx_1}},$$

and in these formulae two pairs of variables $[x_1, y_1]$ and $[x_4, y_4]$ can be changed by any other pairs $[x_j, y_j]$ and $[x_k, y_k]$ provided that $j \neq k$.

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 \equiv \Delta x$, then values $u \equiv \exp(c\cdot\Delta x)$ and $v \equiv \exp(d\cdot\Delta x)$ are roots of the quadratic equation

$$(y_2^2 - y_1 y_3)\cdot\xi^2 + (y_1 y_4 - y_2 y_3)\cdot\xi + (y_3^2 - y_2 y_4) = 0.$$

The initial system of equations has the solution in and only in a case, if the given quadratic equation has two real, positive and not coinciding to each other roots.

6. Function $h + a\cdot e^{cx} + b\cdot e^{dx}$

Let be necessary to interpolate the function $h + a\cdot e^{cx} + b\cdot e^{dx}$ using five paired numbers $\{x_k, y_k\}$, $k = 1,\ldots,5$, i.e. to solve the system of equations

$$h + a\,e^{cx_k} + b\,e^{dx_k} = y_k,\qquad k = 1,\ldots,5$$

with respect to parameters h, a, b, c, d.

The pair of numbers $[c,d]$ can be determined as the root of the system of equations at additional conditions $c \neq d, cd \neq 0$. One of equations of the given system looks like

$$
\begin{aligned}
& y_1 \cdot (e^{cx_3+dx_2} - e^{cx_2+dx_3} + e^{cx_2+dx_4} - e^{cx_4+dx_2} + e^{cx_4+dx_3} - e^{cx_3+dx_4}) + \\
& + y_2 \cdot (e^{cx_1+dx_3} - e^{cx_3+dx_1} + e^{cx_3+dx_4} - e^{cx_4+dx_3} + e^{cx_4+dx_1} - e^{cx_1+dx_4}) + \\
& + y_3 \cdot (e^{cx_2+dx_1} - e^{cx_1+dx_2} + e^{cx_1+dx_4} - e^{cx_4+dx_1} + e^{cx_4+dx_2} - e^{cx_2+dx_4}) + \\
& + y_4 \cdot (e^{cx_1+dx_2} - e^{cx_2+dx_1} + e^{cx_2+dx_3} - e^{cx_3+dx_2} + e^{cx_3+dx_1} - e^{cx_1+dx_3}) = 0,
\end{aligned}
$$

and the second equation can be obtained from the first by replacement in the latest of arbitrary pair of numbers $[x_j, y_j]$ $(j = 1,...,4)$ by $[x_5, y_5]$.

Parameters h, a, b are determined by ratios

$$
\begin{aligned}
a &= \frac{1}{D}\left(y_1 \cdot (e^{dx_2} - e^{dx_3}) + y_2 \cdot (e^{dx_3} - e^{dx_1}) + y_3 \cdot (e^{dx_1} - e^{dx_2})\right), \\
b &= \frac{1}{D}\left(y_1 \cdot (e^{cx_3} - e^{cx_2}) + y_2 \cdot (e^{cx_1} - e^{cx_3}) + y_3 \cdot (e^{cx_2} - e^{cx_1})\right), \\
h &= \frac{1}{D}\left(y_1 \cdot (e^{cx_2+dx_3} - e^{cx_3+dx_2}) + y_2 \cdot (e^{cx_3+dx_1} - e^{cx_1+dx_3}) + y_3 \cdot (e^{cx_1+dx_2} - e^{cx_2+dx_1})\right),
\end{aligned}
$$

where

$$
D = e^{cx_1+dx_2} + e^{cx_2+dx_3} + e^{cx_3+dx_1} - e^{cx_2+dx_1} - e^{cx_3+dx_2} - e^{cx_1+dx_3},
$$

and in these formulae three pair of variables $[x_1, y_1]$, $[x_2, y_2]$ and $[x_3, y_3]$ can be changed by any other pairs $[x_j, y_j]$, $[x_k, y_k]$ and $[x_L, y_L]$ provided that $j \neq k \neq L$.

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 = x_5 - x_4 \equiv \Delta x$, then values $u \equiv \exp(c \cdot \Delta x)$ and $v \equiv \exp(d \cdot \Delta x)$ are roots of the quadratic equation

$$
\xi^2 + p\,\xi + q = 0,
$$

where

$$
\begin{aligned}
p &= \frac{(y_3 - y_2)(y_3 - y_4) + (y_1 - y_2)(y_4 - y_5)}{(y_3 - y_2)^2 + (y_1 - y_2)(y_4 - y_3)}; \\
q &= \frac{(y_3 - y_4)^2 + (y_3 - y_2)(y_4 - y_5)}{(y_3 - y_2)^2 + (y_1 - y_2)(y_4 - y_3)}.
\end{aligned}
\qquad (3.30)
$$

The initial system of equations has the solution in and only in a case, if the given quadratic equation has two real, positive and not coinciding to each other roots.

7. Function $e^{sx} \cdot (A \cdot \cos(\omega x) + B \cdot \sin(\omega x))$

Let be necessary to interpolate the considered function using four paired numbers $\{x_1, y_1\}$, $\{x_2, y_2\}$, $\{x_3, y_3\}$, $\{x_4, y_4\}$, i.e. to solve the system of equations

$$e^{sx_k} \cdot \left(A \cos(\omega x_k) + B \sin(\omega x_k)\right) = y_k, \qquad k = 1,...,4$$

with respect to parameters A, B, s, ω.

The given interpolation is equivalent to the interpolation of the function $\alpha\, e^{\lambda x} + \beta\, e^{\mu x}$,

where

$$\alpha = \frac{1}{2}(A - iB); \quad \lambda = s + i\omega; \qquad \beta = \frac{1}{2}(A + iB); \quad \mu = s - i\omega; \qquad (3.31)$$

at the same time can be used formulae which are given in Item 6 of the given paragraph.

The pair of numbers $[s, \omega]$ can be determined as the solution of any pair from the following four equations

$$y_1 \cdot e^{-sx_1} \sin(\omega x_2 - \omega x_3) + y_2 \cdot e^{-sx_2} \sin(\omega x_3 - \omega x_1) + y_3 \cdot e^{-sx_3} \sin(\omega x_1 - \omega x_2) = 0;$$
$$y_2 \cdot e^{-sx_2} \sin(\omega x_3 - \omega x_4) + y_3 \cdot e^{-sx_3} \sin(\omega x_4 - \omega x_2) + y_4 \cdot e^{-sx_4} \sin(\omega x_2 - \omega x_3) = 0;$$
$$y_1 \cdot e^{-sx_1} \sin(\omega x_2 - \omega x_4) + y_2 \cdot e^{-sx_2} \sin(\omega x_4 - \omega x_1) + y_4 \cdot e^{-sx_4} \sin(\omega x_1 - \omega x_2) = 0;$$
$$y_1 \cdot e^{-sx_1} \sin(\omega x_3 - \omega x_4) + y_3 \cdot e^{-sx_3} \sin(\omega x_4 - \omega x_1) + y_4 \cdot e^{-sx_4} \sin(\omega x_1 - \omega x_3) = 0$$

at additional condition $\omega \neq 0$.

Parameters A and B are determined by ratios

$$A = \frac{y_1 \cdot e^{-sx_1} \sin(\omega x_4) - y_4 \cdot e^{-sx_4} \sin(\omega x_1)}{\sin(\omega x_4 - \omega x_1)}; \quad B = \frac{-y_1 \cdot e^{-sx_1} \cos(\omega x_4) + y_4 \cdot e^{-sx_4} \cos(\omega x_1)}{\sin(\omega x_4 - \omega x_1)},$$

and, in these formulae, two pairs of variables $[x_1, y_1]$ and $[x_4, y_4]$ can be changed by any other pairs $[x_j, y_j]$ and $[x_k, y_k]$ provided that $j \neq k$.

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 \equiv \Delta x$, then values $\xi_1 \equiv \exp((s + i\omega)\cdot\Delta x)$ and $\xi_2 \equiv \exp((s - i\omega)\cdot\Delta x)$ are roots of the quadratic equation

$$\xi^2 + p\,\xi + q = 0, \tag{3.32}$$

where

$$p = \frac{y_1 y_4 - y_2 y_3}{y_2^{\,2} - y_1 y_3}; \qquad q = \frac{y_3^{\,2} - y_2 y_4}{y_2^{\,2} - y_1 y_3}.$$

The initial system of equations has the solution in and only in a case, if the given quadratic equation has two complex conjugate roots (with nonzero imaginary parts). At the same time

$$s = \frac{1}{\Delta x}\cdot\ln|\xi_1| = \frac{1}{2\,\Delta x}\cdot\ln|q|, \tag{3.33}$$

and the set of possible values of ω can be presented as the union of elements of two sequences $[\omega'_k]$ and $[\omega''_k]$, where

$$\omega'_k = \omega_0 + k\cdot\Delta\omega; \quad \omega''_k = -\omega_0 + (k+1)\cdot\Delta\omega; \quad \Delta\omega = 2\pi/|\Delta x|;$$
$$\omega_0 = \left|\frac{\arg(\xi_1)}{\Delta x}\right| = \frac{\Delta\omega}{4} + \frac{1}{|\Delta x|}\cdot\arctan\left(p\cdot(4q - p^2)^{-1/2}\right). \tag{3.34}$$

8. Function $h + e^{sx}\cdot(A\cdot\cos(\omega x) + B\cdot\sin(\omega x))$

Let be necessary to interpolate the considered function using five paired numbers $\{x_k, y_k\}$, $k = 1,...,5$, i.e. to solve the system of equations

$$h + e^{sx_k}\cdot\left(A\cos(\omega x_k) + B\sin(\omega x_k)\right) = y_k, \qquad k = 1,...,5$$

with respect to parameters h, A, B, s, ω.

The given interpolation is equivalent to the interpolation of the function

$$h + \alpha\, e^{\lambda x} + \beta\, e^{\mu x},$$

where α and β are determined by ratios (3.31), at the same time can be used formulae, brought in Item 7 of the given paragraph.

The pair of numbers $[s,\omega]$ can be determined as the root of the system of equations at additional condition $\omega \neq 0$. One of equations of the given system looks like

$$y_1 \cdot (e^{s(x_3+x_2)} \sin(\omega x_3 - \omega x_2) + e^{s(x_2+x_4)} \sin(\omega x_2 - \omega x_4) + e^{s(x_4+x_3)} \sin(\omega x_4 - \omega x_3)) +$$
$$+ y_2 \cdot (e^{s(x_1+x_3)} \sin(\omega x_1 - \omega x_3) + e^{s(x_3+x_4)} \sin(\omega x_3 - \omega x_4) + e^{s(x_4+x_1)} \sin(\omega x_4 - \omega x_1)) +$$
$$+ y_3 \cdot (e^{s(x_2+x_1)} \sin(\omega x_2 - \omega x_1) + e^{s(x_1+x_4)} \sin(\omega x_1 - \omega x_4) + e^{s(x_4+x_2)} \sin(\omega x_4 - \omega x_2)) +$$
$$+ y_4 \cdot (e^{s(x_1+x_2)} \sin(\omega x_1 - \omega x_2) + e^{s(x_2+x_3)} \sin(\omega x_2 - \omega x_3) + e^{s(x_3+x_1)} \sin(\omega x_3 - \omega x_1)) = 0,$$

and the second can be obtained from the first by replacement in the latest of arbitrary pair of numbers $[x_j, y_j]$, $j = 1,...,4$, by $[x_5, y_5]$.

Parameters h, A and B are determined by ratios

$$A = \frac{1}{D}\left((y_1 - y_2) \cdot e^{sx_3} \sin(\omega x_3) + (y_2 - y_3) \cdot e^{sx_1} \sin(\omega x_1) + (y_3 - y_1) \cdot e^{sx_2} \sin(\omega x_2)\right),$$
$$B = \frac{1}{D}\left((y_2 - y_1) \cdot e^{sx_3} \cos(\omega x_3) + (y_3 - y_2) \cdot e^{sx_1} \cos(\omega x_1) + (y_1 - y_3) \cdot e^{sx_2} \cos(\omega x_2)\right),$$
$$h = \frac{1}{D}\left(y_1 \cdot e^{s(x_2+x_3)} \sin(\omega x_2 - \omega x_3) + y_2 \cdot e^{s(x_3+x_1)} \sin(\omega x_3 - \omega x_1) + y_3 \cdot e^{s(x_1+x_2)} \sin(\omega x_1 - \omega x_2)\right),$$

where

$$D = e^{s(x_1+x_2)} \sin(\omega x_1 - \omega x_2) + e^{s(x_2+x_3)} \sin(\omega x_2 - \omega x_3) + e^{s(x_3+x_1)} \sin(\omega x_3 - \omega x_1),$$

and, in these formulae, three pairs of variables $[x_1, y_1]$, $[x_2, y_2]$ and $[x_3, y_3]$ can be changed by any other pairs $[x_j, y_j]$, $[x_k, y_k]$ and $[x_L, y_L]$ provided that $j \neq k \neq L$.

If values of the argument are equidistant from each other, i.e. $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 = x_5 - x_4 \equiv \Delta x$, then values $\xi_1 \equiv \exp((s + i\omega) \cdot \Delta x)$ and $\xi_2 \equiv \exp((s - i\omega) \cdot \Delta x)$ are roots of the quadratic equation (3.32), where p and q are determined by ratios (3.30).

The initial system of equations has the solution in and only in a case, if the given quadratic equation has two complex conjugate roots (with nonzero imaginary parts). At the same time s is calculated by (3.33), and the set of every possible values of ω can be presented as union of elements of two sequences $[\omega'_k]$ and $[\omega''_k]$, where ω'_k, ω''_k, ω_0 and $\Delta\omega$ are determined by ratios (3.34).

3.4.3. Solution of Transcendental Equations of Special Types

The considered below methods of solving of different transcendental equations can be used in many applications. In particular, these methods are used in the problems of interpolation of nonlinear functions of different types considered in the present section.

1. Equation containing sum two exponents.

Let's consider the equation $f(x)=h$, where

$f(x)=a\cdot e^{cx}+b\cdot e^{dx}$,

at $abcd\neq 0$.

Below different methods of determination of boundaries and initial estimates for roots of this equation are considered depending on signs of parameters a, b, c, d. When any number which can be used as initial approach at solving of the equation $f(x)-h=0$ by iterative Newton method is pointed, monotonous convergence of the corresponding iterative sequences to the required root is guaranteed.

a) $ab>0$ and $cd>0$.

At $ha>0$ the function $f(x)-h$ has unique zero x_z belonging to the open interval with boundaries

$$\frac{1}{c}\ \ln\left(\frac{h}{a+b}\right) \text{ and } \frac{1}{d}\ \ln\left(\frac{h}{a+b}\right).$$

In the case $c>0$ and $d>0$ the right boundary of this interval, and in the case $c<0$ and $d<0$ – its left boundary, can be used as the initial approach at solving of the equation $f(x)-h=0$ by Newton iterative method.

At $ha\leq 0$ the function $f(x)-h$ has no zeros.

b) $ab>0$ and $cd<0$.

Let x_0 is the point of extremum of the function and $y_0=f(x_0)$; in the considered case $\operatorname{sign} y_0=\operatorname{sign} a=\operatorname{sign} b$.

At $h/y_0>1$ the function $f(x)-h$ has two zeros x_{z1} and x_{z2}, between which there is the number x_0. Both zeros belong to the open interval with boundaries

$$(1/c)\cdot\ln(h/a) \text{ and } (1/d)\cdot\ln(h/b).$$

Each of these boundaries can be used as initial estimate to the nearest root of the equation $f(x)-h=0$ at solving of this equation by Newton iterative method.

At $h/y_0=1$ the function $f(x)-h$ has one zero coinciding with x_0.

At $h/y_0<1$ the function $f(x)-h$ has no zeros.

c) $ab<0$ and $cd>0$.

Let x_0 is the point of extremum of the function; $y_0=f(x_0)$ and x_{inf} is an abscissa of point of inflection of plot of the function;

$$x_H=\frac{\ln(-a/b)}{d-c}$$

is the point in which $f(x)$ reduces to zero. In the considered case $\operatorname{sign} y_0=\operatorname{sign}(a\ (d-c))=\operatorname{sign}(b\ (c-d))$.

At $h/y_0\le 0$ the function $f(x)-h$ has one zero x_z belonging to the open interval which boundaries are numbers

$$-\frac{1}{d}\ \ln\left(\frac{b}{h-a}\right) \quad \text{and} \quad \frac{1}{c-d}\ \ln\left(\frac{b}{h-a}\right) \qquad (\text{at } c<d)$$

or

$$-\frac{1}{c}\ \ln\left(\frac{a}{h-b}\right) \quad \text{and} \quad \frac{1}{d-c}\ \ln\left(\frac{a}{h-b}\right) \qquad (\text{at } c>d).$$

Besides the number x_H is the lower bound for x_z (at $c>0$ and $d>0$) or the upper bound for x_z (at $c<0$ and $d<0$). Any upper bound for x_z (at $c>0$ and $d>0$) or any lower bound for x_z (at $c<0$ and $d<0$) can be taken as an initial estimate to x_z at solving of the equation $f(x)-h=0$ by Newton iterative method.

At $0<h/y_0<1$ the function $f(x)-h$ has two zeros x_{z1} and x_{z2}, between which it is the number x_0. The point $\{x_0,y_0\}$ divides the plot of the function $y=f(x)$ on two branches, one of which at $x\to\infty$ asymptoticly approachs to the abscissa axis, and another leaves in infinity. Let's consider for definiteness that the first of these branches contains the point $\{x_{z1},h\}$, and the second – the point $\{x_{z2},h\}$. Then x_{z2} belongs to the open interval which boundaries are the numbers x_0 and x_H. The numbers x_{inf} and x_H can be used as

initial estimates, respectively, to x_{z1} and x_{z2} at solving the equation $f(x)-h=0$ by Newton iterative method.

At $h/y_0=1$ the function $f(x)-h$ has one zero coinciding with x_0.

At $h/y_0>1$ the function $f(x)-h$ has no zeros.

d) $ab<0$ and $cd<0$.

The function $f(x)-h$ for any h has one zero x_z belonging to the open interval which boundaries are numbers

$$-\frac{1}{d}\ \ln\left(\frac{b}{h-a}\right) \text{ and } \frac{1}{c-d}\ \ln\left(\frac{b}{h-a}\right)\ (\text{at } hb>0)$$

or

$$-\frac{1}{c}\ \ln\left(\frac{a}{h-b}\right) \text{ and } \frac{1}{d-c}\ \ln\left(\frac{a}{h-b}\right)\ (\text{at } ha>0).$$

2. Equation containing sum of several exponents.

Let it is required to determine real solutions of the equation $f(x)=0$, where

$$f(x)=\sum_{k=0}^{n} a_k\ e^{c_k x};$$

$$a_k\neq 0;\ c_0<c_1<\ldots<c_n.$$

a) *Boundaries of zeros.* Taking into account that considered function can be presented as follows

$$f(x)=a_n\ e^{c_n x}\left(1+\sum_{k=0}^{n-1}\frac{a_k}{a_n}e^{-(c_n-c_k)x}\right)=a_0\ e^{c_0 x}\left(1+\sum_{k=1}^{n}\frac{a_k}{a_0}e^{(c_k-c_0)x}\right),$$

We will obtain the following rules of determination of boundaries of zeros of these function:

If for some number $s>0$ it takes place

$$\sum_{k=0}^{n-1}\left|\frac{a_k}{a_n}\right|\ e^{-(c_n-c_k)s}<1,$$

then s is an upper bound of all real zeros of the function $f(x)$; at $x > s$ it takes place $\operatorname{sign} f(x) = \operatorname{sign} a_n$.

If for some number $s > 0$ it takes place

$$\sum_{k=1}^{n} \left| \frac{a_k}{a_0} \right| e^{-(c_k - c_0)s} < 1,$$

then $-s$ is a lower bound of all real zeros of the function $f(x)$; at $x < -s$ it takes place $\operatorname{sign} f(x) = \operatorname{sign} a_0$.

In both cases it is possible to appropriate to the parameter s the initial value equal to zero and then increase this parameter by some constant (for example, by 1) until the required inequality will be executed.

b) *Algorithm of determination of zeros.* The offered below algorithm of determination of zeros of the function $f(x)$ is based on the following relation for the derivative of this function:

$$e^{c_m x} \frac{d}{dx}\left(e^{-c_m x} f(x) \right) = \sum_{k \neq m} a_k \ (c_k - c_m)\, e^{c_k x} \qquad (m = 0, ..., n).$$

The right side of the latter equality contains the number of exponents by one less than the function $f(x)$ and hence, the problem of determination of its zeros appears easier than one for the function $f(x)$.

Real roots of the equation $f(x) = 0$ can be determined by means the following algorithm:

Elements of the triangular matrix

$$\begin{bmatrix} a_0^{(0)}, & 0, & ..., & 0 \\ a_0^{(1)}, & a_1^{(1)}, & ..., & 0 \\ ... & ... & ... & ... \\ a_0^{(n)}, & a_1^{(n)}, & ..., & a_n^{(n)} \end{bmatrix}$$

are determined by means of relations:

$$a_k^{(n)} = a_k \qquad (k = 0, ..., n);$$

$$a_k^{(j-1)} = a_k^j \cdot (c_k - c_j) \qquad (j = 1, ..., n;\ k = 0, ..., j-1).$$

Then successively for various values $j = 1,..,n$ real zeros $x_1^{(j)}$, ..., $x_{n_j}^{(j)}$ of the functions

$$f^{(j)}(x) = \sum_{k=0}^{j} a_k^{(j)} \; e^{c_k x}$$

are determined. Each sequence of such zeros is supposed arranging in increasing order.

At $j = 1$ two cases are possible: at $a_0^{(1)} \cdot a_1^{(1)} < 0$ the function $f^{(1)}(x)$ has unique zero

$$x_1^{(1)} = \frac{1}{c_1 - c_0} \; \ln\left(-a_0^{(1)} / a_1^{(1)}\right);$$

otherwise the function $f^{(1)}(x)$ has no zeros.

At $j > 1$ for determination of zeros of the function $f^{(j)}(x)$ there are used determined earlier zeros of the function $f^{(j-1)}(x)$ and also determined by rules of Item a) lower x_{lo} and upper x_{hi} bounds of required zeros. Each of intervals $[x_{lo}, x_1^{(j-1)}]$, $[x_1^{(j-1)}, x_2^{(j-1)}]$, ..., $[x_{j-2}^{(j-1)}, x_{j-1}^{(j-1)}]$, $[x_{j-1}^{(j-1)}, x_{hi}]$ may contain no more than one zero of the function $f^{(j)}(x)$. If this zero exists then it can be determined by the bisection method or the chord method.

Determination of zeros of the function $f^{(n)}(x)$ solves the task in view.

3.5. Construction of Confidence Intervals for Mathematical Expectations of Random Variables

At solving many theoretical and applied problems, the broad applications have confidence intervals for parameters of probability distribution laws of the investigated phenomena. The quality of the confidence interval is determined by its width for the given coefficient of confidence. There are three basic methods of finding confidence intervals [102] which are based: 1) on the frequency theory of probability; 2) on fiducial distributions; 3) on the theorem of Bayes. The first method uses the asymptotic normality of the first derivative of the logarithm of likelyhood function. According to the theorem of Wilks, for large sampls, this method gives shortest on the average intervals for the certain class of distributions [102] (hereinafter we shall call this method classical). The second method uses fiducial distributions, corresponding to the considered distribution. In the third method, the bounds of the confidence interval are established on the basis of a posteriori distribution of probability of the considered parameter.

One of methods of determination of a confidence interval for mathematical expectation of a random variable below is offered, founded on utilization of serial statisticses [1, 111, 112]. As against above described, this method does not demand the knowledge of other parameters of distribution laws (for example, variance at a normal probability distribution law) at construction of a confidence interval of mathematical expectation [113].

Let x is the random variable, definite in the interval $(-\infty,+\infty)$ with mathematical expectation m and variance σ^2; $\Phi(\dot{x})$ and $p(\dot{x})$ are distribution function and distribution density of the suitable normalized random variable $\dot{x}=(x-m)/\sigma$; $[x_1, x_2,..., x_N]$ is N-dimentional sample;

$$x_{\min} = \min_{1\le j\le N}\{x_j\}; \quad x_{\max} = \max_{1\le j\le N}\{x_j\}.$$

Theorem 3.3. *A confidence interval for the parameter m with the confidence level* $1-\alpha$ *is*

$$[x_{\min} - h_N(\alpha)\cdot(x_{\max}-x_{\min}); x_{\max} + H_N(\alpha)\cdot(x_{\max}-x_{\min})],$$

where the functions $h = h_N(\alpha)$ and $H = H_N(\alpha)$ *are determined by solving equations*

$$\psi(h) = \alpha/2 \text{ and } \Psi(H) = \alpha/2$$

in domain $h > -1$ *and* $H > -1$, *at*

$$\psi(h) = \int_0^\infty N\cdot p(u)\cdot\left(\Phi(u)-\Phi\left(uh/(1+h)\right)\right)^{N-1} du; \tag{3.35}$$

$$\Psi(H) = \int_0^\infty N\cdot p(-u)\cdot\left(\Phi\left(-uH(1+H)\right)-\Phi(-u)\right)^{N-1} du.$$

Proof: Let us consider random variables

$$u \equiv (x_{\min}-m)/\sigma \text{ and } v \equiv (x_{\max}-m)/\sigma.$$

In accordance with [89, 111], their joint distribution density is equal to

$$p_w(u,v) = N(N-1)\cdot p(u)\cdot p(v)\cdot(\Phi(v)-\Phi(u))^{N-2} \text{ at } u \le v.$$

The bounds of the confidence interval are determined from the conditions

$$\mathrm{P}\{x_{\min} - h_N(\alpha)\cdot(x_{\max}-x_{\min}) > m\} = \alpha/2;$$
$$\mathrm{P}\{x_{\max} + H_N(\alpha)\cdot(x_{\max}-x_{\min}) < m\} = \alpha/2$$

(the symbol P means the probability of the event). Inequalities

$$x_{\min} - h\cdot(x_{\max}-x_{\min}) > m \text{ and } x_{\max} + H\cdot(x_{\max}-x_{\min}) < m$$

are equivalent of inequalities

$$v \cdot h/(1+h) < u \text{ and } v < u \cdot H/(1+H);$$

to them there correspond domains D_1 and D_2 on the plane (*uv*), showed in Figure 3.8.

Let us designate by $\psi(h)$ and $\Psi(H)$ the probabilities of these inequalities; then

$$\psi(h) = \int_0^{\infty} \left(\int_{vh/(1+h)}^{v} p_w(u,v)du \right) dv =$$

$$= \int_0^{\infty} N \cdot p(v) \cdot \left(\Phi(v) - \Phi\left(vh/(1+h)\right)\right)^{N-1} dv$$

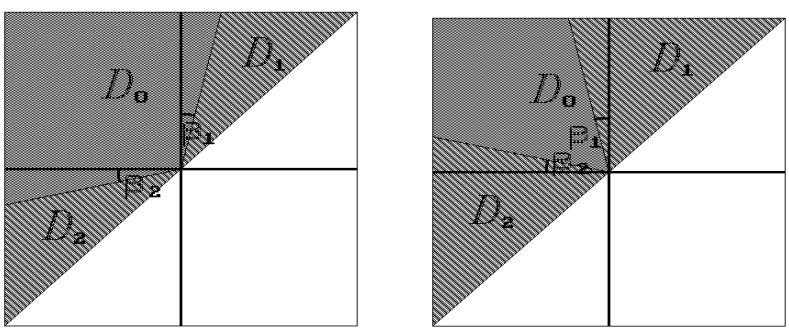
and

$$\Psi(H) = \int_{-\infty}^{0} \left(\int_{u}^{uH/(1+H)} p_w(u,v)dv \right) du =$$

$$= \int_0^{\infty} N \cdot p(-u) \cdot \left(\Phi\left(-uH/(1+H)\right) - \Phi(-u)\right)^{N-1} du,$$

what was necessary to prove.

The coordinate axises are designated by u and v; the region D_0 is bounded by straight lines $v = u \cdot (1+h)/h$ and $v = u \cdot H/(1+H)$; the region D_1 is in upper half-plane between straight lines $v = u$ and $v = u \cdot (1+h)/h$, and region D_2 is in lower half-plane between straight lines $v = u$ and $v = u \cdot H/(1+H)$.



a) h > 0, H > 0; b) h < 0, H < 0.

Figure 3.8. Critical resgions D1, D2 and region of acceptance of hypothesis D0; tg β1 = h/(1+h); tg β2 = H/(1+H).

Let us note that the equations (3.35) do not contain the parameter σ. It takes place because the change of σ corresponds to the change of the scale in Figure 3.8, at which each of domains D_0, D_1 and D_2 does not change its position with regard to the coordinate axises.

For positive values of the argument of functions $\psi(h)$ and $\Psi(H)$ they can also be determined by formulae

$$\psi(h) = \int_0^\infty N \cdot p(u) \cdot \left(\Phi\left(u(1+h)/h\right) - \Phi(u)\right)^{N-1} du \tag{3.36}$$

$$\Psi(H) = \int_0^\infty N \cdot p(-u) \cdot \left(\Phi(-u) - \Phi\left(-u(1+H)/H\right)\right)^{N-1} du.$$

The given ratios can be obtained as follows: let us designate by $\psi'(h)$ the function, equal to the right part of the first equation (3.36), then

$$\psi(h) - \psi'(h) =$$

$$= \int_0^\infty N \cdot \left(p(u) - \frac{h}{1+h} \cdot p\left(uh/(1+h)\right)\right) \cdot \left(\Phi(u) - \Phi\left(uh/(1+h)\right)\right)^{N-1} du =$$

$$= \left(\Phi(u) - \Phi\left(uh/(1+h)\right)\right)^N \Big|_0^\infty = 0.$$

If the function $p(u)$ is even, i.e. symmetrical concerning mathematical expectation, then $\psi(h) = \Psi(H)$ and, accordingly, $h_N(\alpha) = H_N(\alpha)$.

The mentioned below results are valid for symmetrical probability distribution densities.

Let us bring the values of $h_N(\alpha)$ for limiting values of the confidence probability at fixed N: at $\alpha \to 0$, $h_N(\alpha) \to \infty$, and at $\alpha \to 1$, $h_N(\alpha) \to -1/2$.

It is possible to demonstrate the latest ratio as follows: at $h = -1/2$

$$\psi(-1/2) = \int_0^\infty N \cdot p(u) \cdot \left(2\Phi(u) - 1\right)^{N-1} du = \frac{1}{2} \cdot \left(2\Phi(u) - 1\right)^N \Big|_0^\infty = \frac{1}{2}.$$

The values of coefficients $h_N(\alpha) = H_N(\alpha)$ for different N and α at normal and uniform probability distributions with arbitrary variance are presented in Tables 3.2 and 3.4. As it is seen from the tables, at fixed α by increase of the sample size N the function $h_N(\alpha)$ decreases and, since some value of N becomes negative.

The value of N, at transition through which one $h_N(\alpha)$ changes the sign, is possible to calculate as follows: at $h = 0$

$$\psi(0)=\int_0^{\infty} N\cdot p(u)\cdot\left(\Phi(u)-\Phi(0)\right)^{N-1}du=\left(\Phi(u)-\Phi(0)\right)^{N}\Big|_0^{\infty}=\left(\frac{1}{2}\right)^{N}.$$

It is obvious that $\Phi(h)$ is increasing function. Therefore, at $\alpha/2<2^{-N}$, $h_N(\alpha)>0$, and at $\alpha/2>2^{-N}$, $h_N(\alpha)<0$, i.e. the function $h_N(\alpha)$ is negative at $N>\log_2(2/\alpha)$.

Let us consider the limit $h_N(\alpha)$ at $N\to\infty$ for fixed α.

Theorem 3.4. *If the density function* $p(u)$ *is continuum and there is such positive number* u_B *that at* $u>u_B$ *the function* $p(u)/p(bu)$ *decreases and*

$$\lim_{u\to\infty} p(u)/p(bu)=0,\quad \forall b,\ 0\le b<1,$$

then

$$\lim_{N\to\infty} h_N(\alpha)=-\frac{1}{2}. \tag{3.37}$$

It is obvious that the condition of the theorem is valid for normal distribution.

Proof. In accordance with the condition of the theorem the function $p(u)$ is strictly monotonic at $u>u_B$. Let us designate

$$s_{\mathrm{N}}=1+\frac{h_N(\alpha)}{1+h_N(\alpha)}\quad\text{and}\quad u_N=\Phi^{-1}(1-N^{-1/2}),$$

where $\Phi^{-1}(\cdot)$ is the function, inverse of $\Phi(\cdot)$. Let $N>(1-\Phi(u_B))^{-2}$ and, therefore, $u>u_B$, and also $h_N(\alpha)<0$ and, consequently, $0<s_N<1$. Let us divide the integration interval into two subinterval in the expression determining $\psi(h)$; we shall obtain

$$\alpha=2\cdot\psi\left(h_N(\alpha)\right)=\int_0^{u_N}2N\cdot p(u)\cdot\left(\Phi(u)+\Phi(u-u\cdot s_N)-1\right)^{N-1}du+$$

$$+\int_{u_N}^{\infty}2N\cdot p(u)\cdot\left(\Phi(u)+\Phi\left(u-u\cdot s_N\right)-1\right)^{N-1}du\le$$

$$\le \int_0^{u_N} 2N \cdot p(u) \cdot \left(2\Phi(u)-1\right)^{N-1} du +$$

$$+ \int_{u_N}^{\infty} \frac{2p(u)}{p(u)+(1-s_N)\cdot p\left((1-s_N)\cdot u\right)} \cdot \frac{d}{du}\left(\Phi(u)+\Phi(u-u\cdot s_N)-1\right)^N du \le$$

$$\le \int_0^{u_N} \frac{d}{du}\left(2\Phi(u)-1\right)^N du +$$

$$+ \frac{2p(u_N)}{p(u_N)+(1-s_N)\cdot p\left((1-s_N)\cdot u_N\right)} \cdot \int_{u_N}^{\infty} \frac{d}{du}\left(\Phi(u)+\Phi(u-u\cdot s_N)-1\right)^N du =$$

$$= \left(2\Phi(u_N)-1\right)^N +$$

$$+ \frac{2p(u_N)}{p(u_N)+(1-s_N)\cdot p\left((1-s_N)\cdot u_N\right)} \cdot \left(1-\left(\Phi(u_N)+\Phi(u_N-u_N\cdot s_N)-1\right)^N\right) \le$$

$$\le \left(2\Phi(u_N)-1\right)^N + \frac{2}{1+(1-s_N)\cdot p\left((1-s_N)\cdot u_N\right)/\, p(u_N)}.$$

The first term in the right part of the given equality

$$(2\cdot\Phi(u_N)-1)^N = (1-2N^{-1/2})^N \to 0 \quad \text{at} \quad N\to\infty.$$

Let us consider the second term. It is obvious that at $N\to\infty$ the limit of the second term should tend to $\alpha_1 \ge \alpha > 0$. In this case, it should take place $S_N \to 0$. Otherwise, let $S_N \ne 0$, i.e. $0 < S_N < 1$. Then, in accordance with the condition of the theorem, at $N\to\infty$ there will take place $P((1-S_N)\cdot u_N)/P(u_N)\to\infty$, i.e. the second term tends to 0, which contradicts the above-stated inequality. Consequently

$$\lim_{N\to\infty} h_N(\alpha) = \lim_{N\to\infty} -\frac{1-s_N}{2-s_N} = -\frac{1}{2},$$

what was necessary to prove.

Let us note that the condition of the theorem is sufficient, but it is not necessary, since for some widespread distributions, such as, for example, uniform distribution, the condition of the theorem is not fulfilled, but (3.37) takes place.

For the uniform distribution, simple, evident expressions for functions $\psi_N(h)$ and $h_N(\alpha)$ can be obtained:

$$\psi_N(h) = \frac{1}{2}\left(2\,(1+h)\right)^{-N+1}; \quad h_N(\alpha) = \frac{1}{2}\,\alpha^{-1/(N-1)} - 1\ .$$

If the variable x is distributed normally, then at calculation of the function $\psi(h) = \Psi(h)$, it is expedient to use the quadrature formula of Laguerre

$$\psi(h) = \int_0^\infty e^{-x^2/2} \cdot f(x)\, dx = \int_0^\infty e^{-y} \cdot (2y)^{-1/2} f\left(\sqrt{2y}\right) dy \approx$$

$$\approx \sum_{k=1}^{n} w_k \cdot \frac{f\left(\sqrt{2\xi_k}\right)}{\sqrt{2\xi_k}},$$

where

$$f(x) = N \cdot \frac{1}{\sqrt{2\pi}} \cdot \left(\Phi_{norm}(x) - \Phi_{norm}\left(xh/(1+h)\right)\right)^{N-1};$$

$\Phi_{norm}(x)$ is the distribution function of the standardized normal variable; $\xi_k, k = 1,...,n$ are zeros of the polynomial of Laguerre $L_n^{(0)}(x)$ of power n; $w_k = \dfrac{1}{\xi_k \cdot \left(\dot{L}_n^{(0)}(\xi_k)\right)^2}$ are weigh coefficients of the quadrature formula.

If the number of nodal points N take equal to 16, then it provides the accuracy of calculation of negative values of the function $h_N(\alpha)$, by which they are presented in Tables 3.2 and 3.4.

If, at calculation of functions $\psi_N(h)$ and $\Psi_N(h)$, the quadrature formula of Gauss or any other formula of approximate calculation of the integral, for the bounded interval, uses, then, it is obvious that the upper bound of integration must be replaced by finit number. Let us designate by $\rho'(v)$ and $\rho''(v)$ the errors of calculation of functions $\psi_N(h)$ and $\Psi_N(H)$, respectively, caused by replacement of the upper bound of integration by number v. Then

$$0 < \rho'(v) < \left(\frac{q \cdot p(qv)}{p(v)} - 1\right)^{-1} \cdot \left(\Phi(v) - \Phi(qv)\right)^N \quad (q > 0);$$

$$0 < \rho'(v) < \left(1 - \frac{q \cdot p(qv)}{p(v)}\right)^{-1} \cdot \left(1 - \left(\Phi(v) - \Phi(qv)\right)^N\right) \quad (q < 0);$$

$$0 < \rho''(V) < \left(\frac{Q \cdot p(-QV)}{p(-V)} - 1 \right)^{-1} \cdot \left(\Phi(-QV) - \Phi(-V) \right)^N \quad (Q > 0);$$

$$0 < \rho''(V) < \left(1 - \frac{Q \cdot p(-QV)}{p(-V)} \right)^{-1} \cdot \left(1 - \left(\Phi(-QV) - \Phi(-V) \right)^N \right) \quad (Q < 0),$$

where $q \equiv h/(1+h)$; $Q \equiv H/(1+H)$. These formulae allow to determine functions $\psi_N(h)$ and $\Psi_N(H)$ with required accuracy. Let us note that if for normal distribution the value of the parameter v, provided the condition $|\rho'(v)| < 1 \cdot 10^{-8}$, is equal to $2 \div 7$, then for the lognormal distribution, at the same accuracy, it is necessary to take $v = 30 \div 500$.

Table 3.4. Values of the coefficients $h_N(\alpha)$

	Uniform distribution		
$N\backslash\alpha$	0.10	0.05	0.02
2	4.0000	9.0000	24.000
3	0.5811	1.2361	2.5355
4	0.0772	0.3572	0.8420
5	–0.1109	0.0574	0.3296
6	–0.2076	–0.0897	0.0934
7	–0.2661	–0.1762	–0.0403
8	–0.3053	–0.2329	–0.1257
9	–0.3332	–0.2729	–0.1847
10	–0.3542	–0.3025	–0.2278
11	–0.3705	–0.3254	–0.2606
12	–0.3836	–0.3435	–0.2865
13	–0.3942	–0.3582	–0.3073
14	–0.4031	–0.3704	–0.3244
15	–0.4106	–0.3807	–0.3388
16	–0.4170	–0.3895	–0.3510
17	–0.4226	–0.3970	–0.3615
18	–0.4275	–0.4037	–0.3706
19	–0.4318	–0.4095	–0.3786
20	–0.4356	–0.4146	–0.3857
21	–0.4390	–0.4192	–0.3920
22	–0.4421	–0.4233	–0.3976
23	–0.4448	–0.4271	–0.4027
24	–0.4474	–0.4304	–0.4073
25	–0.4497	–0.4335	–0.4115
26	–0.4518	–0.4363	–0.4153
27	–0.4537	–0.4389	–0.4188
28	–0.4555	–0.4413	–0.4220
29	–0.4571	–0.4435	–0.4250
30	–0.4587	–0.4456	–0.4278
40	–0.4696	–0.4601	–0.4472

50	–0.4759	–0.4685	–0.4584
60	–0.4801	–0.4740	–0.4657
70	–0.4830	–0.4778	–0.4708
80	–0.4852	–0.4807	–0.4746
90	–0.4869	–0.4829	–0.4775
100	–0.4882	–0.4846	–0.4798
200	–0.4942	–0.4924	–0.4901
300	–0.4961	–0.4950	–0.4934

Let us consider the case when the graph of the distribution density of the variable x forms the trapezoid with the axis of abscissa, the divisionof the lengthes of upper and lower bases of which is equal to λ. Such kind of distribution we shall call generalized trapezoidal. The parameter λ, it is clear, satisfys the inequality $0 \le \lambda \le 1$. In particular, at $\lambda = 1$, x has the uniform distribution, at $\lambda = 0$ - triangle, and at $\lambda = 1/3$ - trapezoidal.

For obtaining explicit expressions for the function $\psi_N(h)$ at $\lambda < 1$ can be used formula [225]

$$\int z^{s-1} \cdot (1 - \beta z^{\kappa})^{\alpha} \, dz = s^{-1} \cdot z^{s} \cdot {}_2F_1(-\alpha, s/\kappa; s/\kappa + 1; \beta z^{\kappa})$$

($s \neq 0$; $\kappa \neq 0$; $s/\kappa \neq 0, -1, -2, \cdots$), by which can be obtained

$$\int (a_0 + a_1 z + a_2 z^2)^s \, dz =$$

$$= \frac{1}{2a_2}\left(a_0 - \frac{a_1^2}{4a_2}\right)^s (a_1 + 2a_2 z) \cdot {}_2F_1\left(-s, \frac{1}{2}; \frac{3}{2}; \frac{(a_1 + 2a_2 z)^2}{a_1^2 - 4a_0 a_2}\right)$$

and

$$\int z \cdot (a_0 + a_1 z + a_2 z^2)^s \, dz = \frac{(a_0 + a_1 z + a_2 z^2)^{s+1}}{2a_2(s+1)} -$$

$$- \frac{a_1}{2a_2^2}\left(a_0 - \frac{a_1^2}{4a_2}\right)^s (a_1 + 2a_2 z) \cdot {}_2F_1\left(-s, \frac{1}{2}; \frac{3}{2}; \frac{(a_1 + 2a_2 z)^2}{a_1^2 - 4a_0 a_2}\right).$$

In general case, for arbitrary value of λ, the expression for the function $\psi_N(h)$ is cumbersome and, therefore, they are not brought here. However they are significantely simplified at $\lambda = 0$, i.e. when x has triangualar distribution, and it takes the kind:

at $h > 0$

$$\psi_N(h) = \frac{1}{2(1+2h)\cdot\left(2(1+h)^2\right)^{N-1}} +$$

$$+ \frac{4Nh}{\left(2(1+2h)\right)^{N+1}}\cdot\left((1+h)\cdot V_0 + h\cdot {}_2F_1\left(-N+1, \frac{1}{2}; \frac{3}{2}; \frac{h^2}{(1+h)^2}\right)\right);$$

at $h < 0$

$$\psi_N(h) = \frac{1}{2(1-2h^2)(1+2h+2h^2)}\cdot\left(\frac{1-2h^2}{2(1+h)^2}\right)^{N-1} +$$

$$+ \frac{4Nh(1+2h)}{\left(2(1+2h+2h^2)\right)^{N+1}}\cdot\left((1+h)\cdot V_0 + h(1+2h)\cdot {}_2F_1\left(-N+1, \frac{1}{2}; \frac{3}{2}; \left(\frac{h(1+2h)}{1+h}\right)^2\right)\right),$$

where

$$V_0 = {}_2F_1(-N+1, 1/2; 3/2; 1) = \prod_{k=1}^{N-1}\frac{k}{k+1/2}.$$

It is preferable to compute the values of the hypergeometric polynomial $B_N \equiv {}_2F_1(-N, \alpha; \gamma; z)$ with the help of recurrent formula

$$B_{N+1} = (\gamma+N)^{-1}\left((\gamma+2N-Nz-\alpha z)\cdot B_N - N(1-z)\cdot B_{N-1}\right).$$

If it computs by summation of the hypergeometric series then at big N the error of computation could be big, as neighbouring items of this series have different signs and their absolute values are considerably big than the sum.

In Figure 3.9 and 3.10 are given the dependences of the length of the confidence interval, computed by classical and above brougth methods, respectively, on the sample size at fixed variance of observation results and on standard deviation at fixed size of sample for normal distribution. In Figure 3.11 and 3.12, 3.13 and 3.14, also 3.15 and 3.16 are given the analogous dependences, for lognormal, triangular and uniform laws of probability distribution, respectively.

The computation of the length of one value of the confidence interval is realized by averaging triple computation of its value on the basis of three independent sampls of necessary sizes for given parameters.

From these dependences it is seen that for normal, lognormal and triangular distributions the classical method gives the best result. For the normal distribution this must true in accordance with the theorem of Wilks [102], since in this case the likelyhood function is distributed normally. For the uniform distribution, the offered method, in which the

coefficient $h_N(\alpha)$ is calculated by probability distribution laws of the random variables, gives much best result, than classical method. If draw the graphs, similar to the shown in Figure 3.9 -3.16 for generalized trapezoidal distributions at different values of the parameters λ, it is possible to reveal that at $\lambda > 0.4$, the offered method gives the best result than classical.

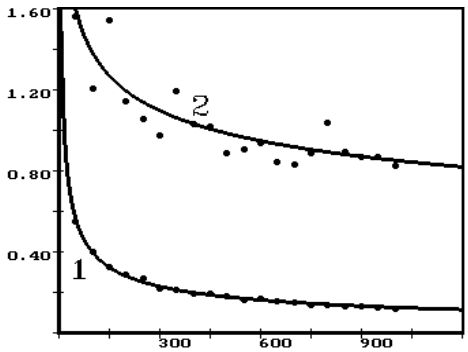


Figure 3.9. Dependence of the length of the confidence interval on the sample size for normal probability distribution law at $m = 0, \sigma = 1$; 1 - classic method; 2 - new method.

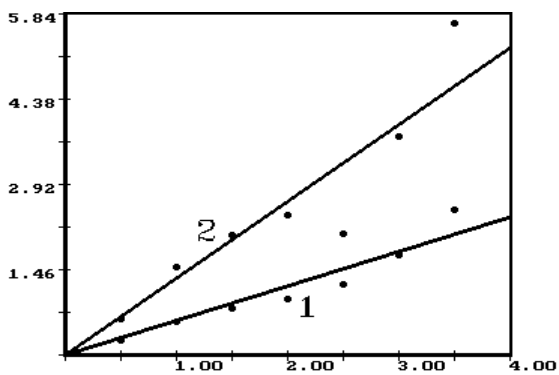


Figure 3.10. Dependence of the length of the confidential interval on standard deviation for normal probability distribution law of at sample size $N = 50$; 1 - classic method; 2 - new method.

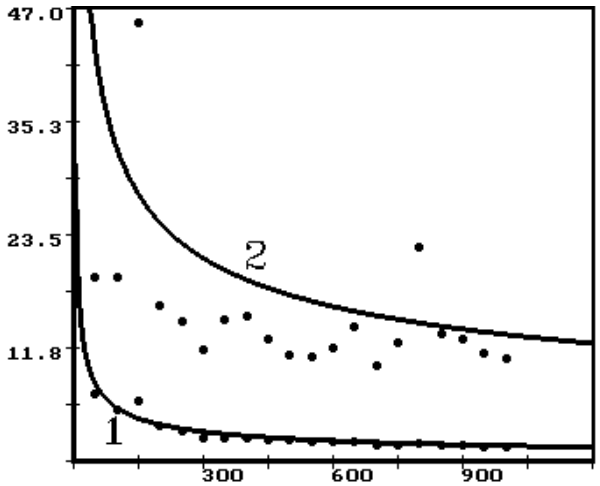


Figure 3.11. Dependence of the length of the Confidential interval on the sample size for lognormal probability distribution law at $a = 3, \sigma = 0.5$; 1 - classic method; 2-new method.

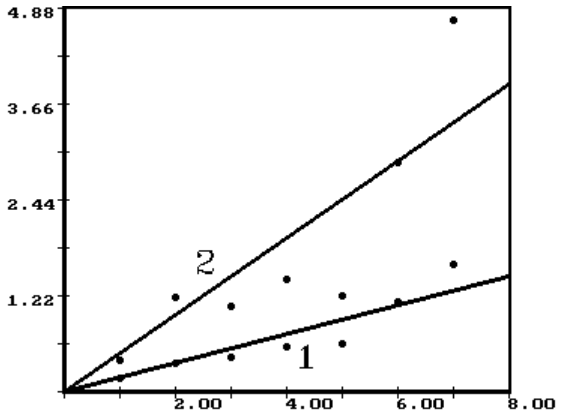


Figure 3.12. Dependence of the length of the confidential interval on the parameter e^a, proportional to the standard deviation, for lognormal probability distribution law at $\sigma = 0.5$ and sample size $N = 50$; 1- classic method; 2- new method.

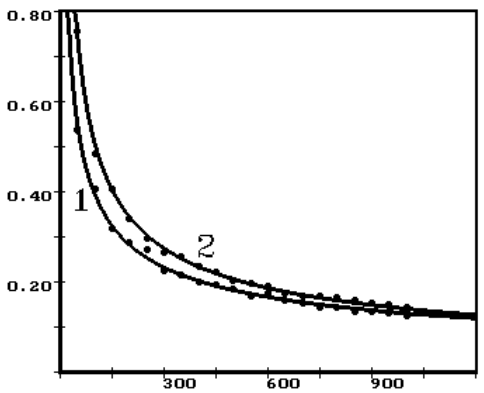


Figure 3.13. Dependence of the length of the confidential interval on the size of sample for triangular probability distribution law at $a = 0$, $b = 5$; 1-classic method; 2-new method.

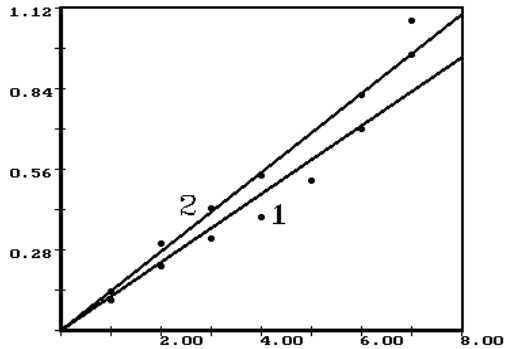


Figure 3.14. Dependence of the length of the confidential interval on the length of domain interval of the random variable for triangular probability distribution law at sample size $N = 50$; 1 - classic method; 2-new method.

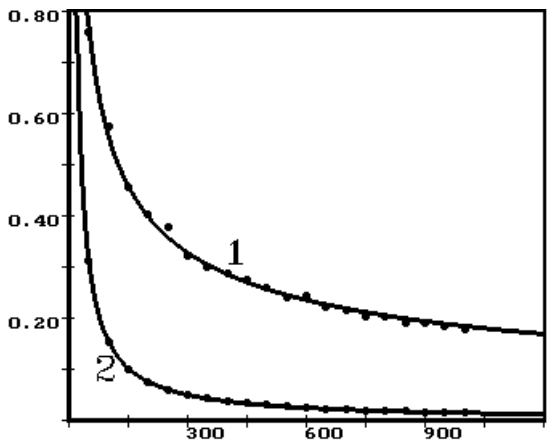


Figure 3.15. Dependence of the length of the confidential interval on sample size for uniform probability distribution law at $a = 0$, $b = 5$; 1 - classic method; 2 – new method.

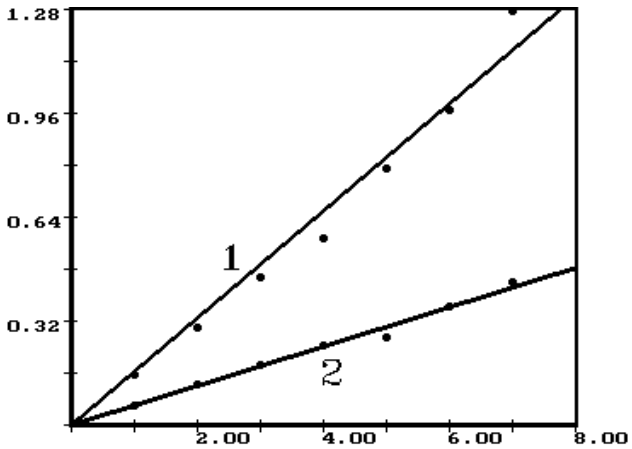


Figure 3.16. Dependence of the length of the confidence interval on the length of domain interval of random variable for uniform probability distribution law at sampl size $N = 50$; 1 - classic method; 2- new method.

Thus, the offered method, except of simplicity of computation, gives the best result than the classical method for the construction of the confidence interval of mathematical expectation of the random variable, if probability distribution of the latest considerably differs from normal.

3.6. IMITATIVE MODELING OF FORMATION OF THE QUALITY OF SEWAGES

The formation of quality of natural waters is rather complex problem. Among the numerous factors, stipulating their condition, it is necessary to single out industrial flows. In order to protect natural waters from the pollution by industrial lfows, they build expensive refining facilities and systems of monitoring of sewages. The efficiency of capital investment depends on the optimality of the accepted designing solutions, in particular, from the calculation of powers of refining facilities, from the rational selection of the equipment of monitoring and, also, from the quality of made decisions in the process of exploitation of refining facilities, from maximum application of their capabilities. For the successful solution of these problems, the large value has the knowledge of the process of formation of the quality of sewages, the ability to predict its development in time with taking into account all possible critical situations, arising in the process of operation of the enterprise [114]. Imitative models of formation of the quality of sewages enable to predict the quality of sewages in dynamics, depending on the given operational mode of the enterprise, not breaking a normal mode of its operation. The following initial information is necessary for their making [1]: the detailed scheme of inter disposition of pollution sources, connected by sewer system of the given enterprise; water expense for each pollution source and the concentration of dropping ingredients in all possible technological modes of operation; working models of transportation of polluting ingredients on considered section of sewer system; the kind and the character of the random component of the pollution process for sources of droppings.

Imitative models of formation of quality of sewages, except of indicated, enable us [1]: to control indirectly the activity of autoanalyzers of the water quality by comparison of simulation results and measured values of the same parameters; at temporary disabling any of measurement channel to fill the gaps in measurements of the given parameter, to calculate concentrations of controled ingredients in an uncotroled point of water object in accordance with the conditions of dropping of sewages by pollution sources (it allows to reduce up to the minimum the necessary number of measurement facilities, necessary for the control of water object with the given reliability); to calculate Maximum Allowable Discharge (MAD) for objects of pollution with the purpose of the maintenance of concentrations of controled ingredients in bounds of maximum allowable concentration (MAC); to predict concentrations of controled ingredients in a given point of water object depending on the conditions of discharge of sewages by dropping sources; to find out sources of emergency pollution; to test, to coordinate and to optimize of technical, informational-program and mathematical supports of the developed automated quality monitoring system of the natural water, which considerably increases the efficiency of such developments and reduces up to minimum the time for their introduction in real object.

In order to unify algorithms and programs, imitative models should be developed by modular-modulus principle with optimum separation of functions among the blocks, permitting to imitate different processes of pollution by the rearrangement of the order of the fulfilment and minimum replacement of developed blocks.

The existence in imitative models of the following basic blocks seems to be expedient [1]: generation of the technological operational modes of pollution sources, i.e. generation of the block of control; realization of mathematical models of the transport of pollutants in the water; generation of multidimensional stochastic processes, having the given nature; generation of random numbers by the given probability distribution law.

Developed by the author of the present book imitative model of the pollution process of the sewage of Odessa Nitrogen Factory is given below [1, 115]. The simulation of pollution process is considered on the example of the most typical segment of the factory, for simplicity of presentation. In Figure 3.17 is given schematic view of the modeled segment of Odessa Nitrogen Factory. Here directions of arrows, connecting pollution sources *(S1, ...,S5)* and an autoanalyzer of water quality, correspond to the direction of the stream of water; T_1, T_2, T_3, T_4 are nodal points of the system of drains; *S1, S2* drop Ammonia; *S3, S4* drop Ammonia and Carbamidum and *S5* drops Ammonia, Carbamidum, Nitrogennitrite, Nitrogennitrate, Natrii phosphases. The program structure of imitative model of the pollution process of water is given in Figure 3.18. By arrow is shown the direction of circulation among program blocks.

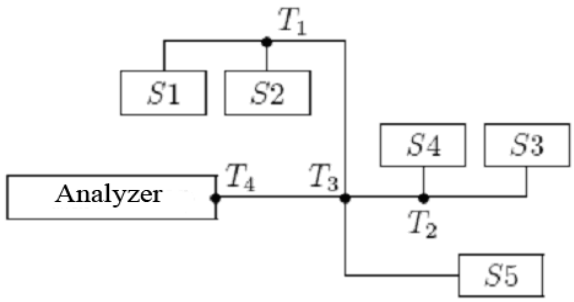


Figure 3.17. Schematic view of modeling segment of Odessa Nitrogen Factory.

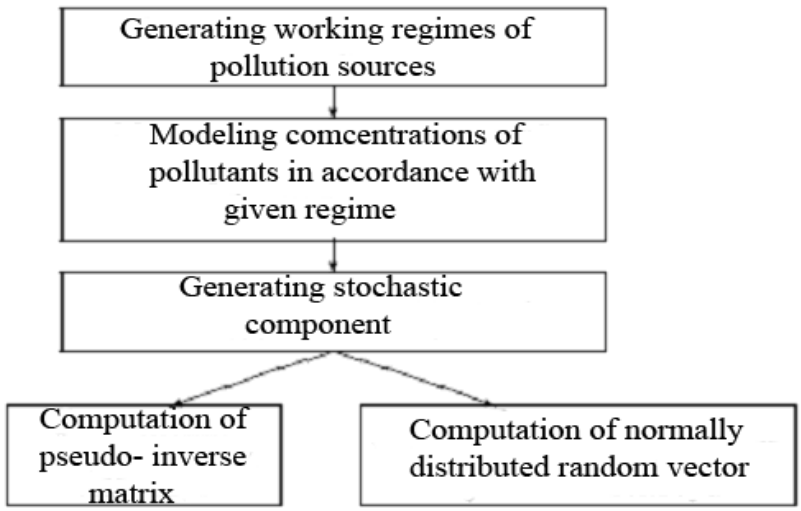


Figure 3.18. Program structure of imitative model of water pollution process.

As almost any real process, the formation of the quality of sewages is a dynamic and stochastic system. As dynamic mathematical models of transportation of pollutants in water there are used the models which are taking into account only processes of the dilution and a self-purification [116]:

$$y_p^k(t) = \begin{cases} \sum_{j=1}^{q_k} y_{p,j}(t-\tau_j) + x_p(t) \;\; at \;\; p=1; \\ \dfrac{1}{\sum_{j=1}^{q_k} y_{1,j}} \left[\sum_{j=1}^{q_k} y_{1,j}(t-\tau_j) \times y_{p,j}(t-\tau_j) \right] + x_p(t) \;\; at \;\; p=2,...,m, \end{cases}$$

where $y_1^k(t)$ is the volume of water in k th knot; $y_p^k(t),\ \ p=2,...,m$ is the concentration of p th ingredient in k th knot; q_k is the number of dropsources, participating in the formation of water quality in k th knot; $y_{p,j}(t)$ is the concentration of p th ingredient, droping by j th object of drop; τ_j is the time of runing of the water from j th object of dropings up to k th knot; $x_p(t)$ is the stochastic component of the concentration of p th ingredient.

It is known [117] that the Markov's model is the best for hydrological data. It is supposed that it is also suitable for the data of the pollution of water. Realized by us investigation by natural data of Odessa Nitrogen Factory and the river Kura has confirmed this supposition.

Therefore in offered below models, the stochastic component of concentration of pollutants $x(t)=(x_1(t),...,x_m(t))$ is modelled by the method of group simulation of multivariate normal Markov processes with given depth of connectivity (see paragraph 3.7).

In the block of generation of technological modes of operation of pollution sources, the set of weight coefficients of concentration of dpopping ingredients from pollution sources $K=(k_1,...,k_5)$ are formed. Elements of the vector K satisfies to the ratio $0\le k_i\le 1$. The case $k_i=0$ corresponds to waying out of a situation, i.e. to switching-off of the suitable pollution source; $k_i=1$ corresponds to the maximum pollution by i th pollution source. From Figure 3.19, it is seen that as input data for both the given block and the full program of imitative model of the pollution process are: M - the number of modelled ingredients; M_1 - the number of pollution sources; N_1 - the number of modelled modes of operational of pollution sources; K_N - the number of analyzers of the quality of controlled water; N - the depth of connectivity of the modelled Markov process; $a_i, i=1,...,L$ - the concentration of Ammonia for i th pollution source; L -the number of pollution sources, dropping the Ammonia; $b_i, i=1,...,L_1$ - the concentration of Carbamidum for i th pollution source; L_1 the number of pollution sources, dropping the Carbamidum; c the concentration of Phosphate; d the concentration of Nitrogennitrite; e the concentration of Nitrogennitrate; q_i, $i=1,...,M$, - water expense for i -th pollution source; $\tau_i, i=1,...,M$, - the time, for which water runs from i th pollution source up to analyzer (T_4); $K^2_{i>j}, i=1,...,N_1$, $j=1,...,M_1$, - the matrix of giving of modes of operational of pollution sources; n_1 - the step of discreted simulation of pollution process; t^* - the time of the first change of the condition of pollution process; h_t^* - the step of change of condition of the pollution process; T - maximum time of generation of pollution process; $R_{i>j,i}$, $i=1,...,M$, $j=1,...,M$, $l=1,...,N$, intercovariation matrix of stochastic components of concentration of the pollutants; $R0_{i,j}$, $i=1,...,M$, $j=1,...,K_N$ dispersion matrix of stochastic components of

concentrations of the pollutants; IND_i, $i = 1,..., K_N$ elements of the set, obtaining values 0 or 1. As a result of the work of this block is the set $K1_i$, $i = 1,..., M_1$, - current values of weight coefficients for concentrations of pollutants, determining technological modes of operation of the suitable pollution sources.

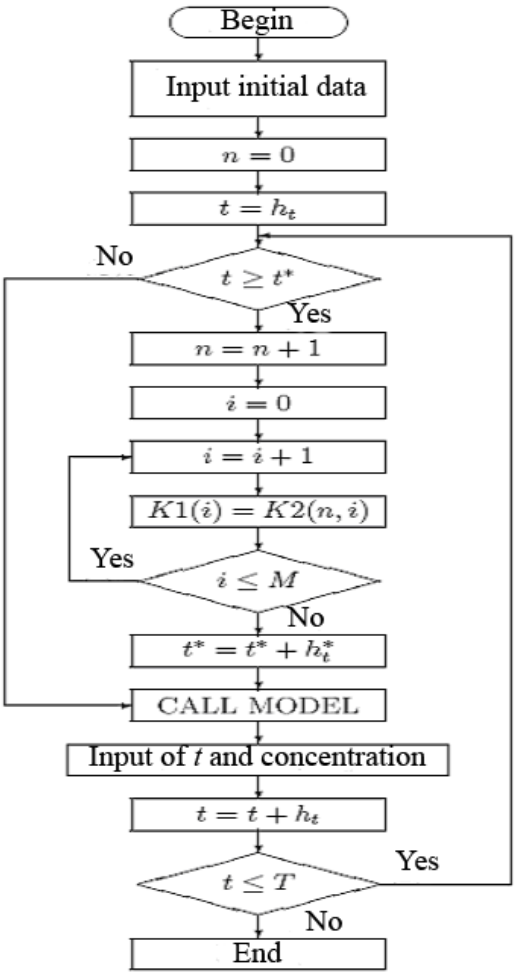


Figure 3.19. The bookkeeping scheme of the algorithm of simulation of modes of operation of pollution sources.

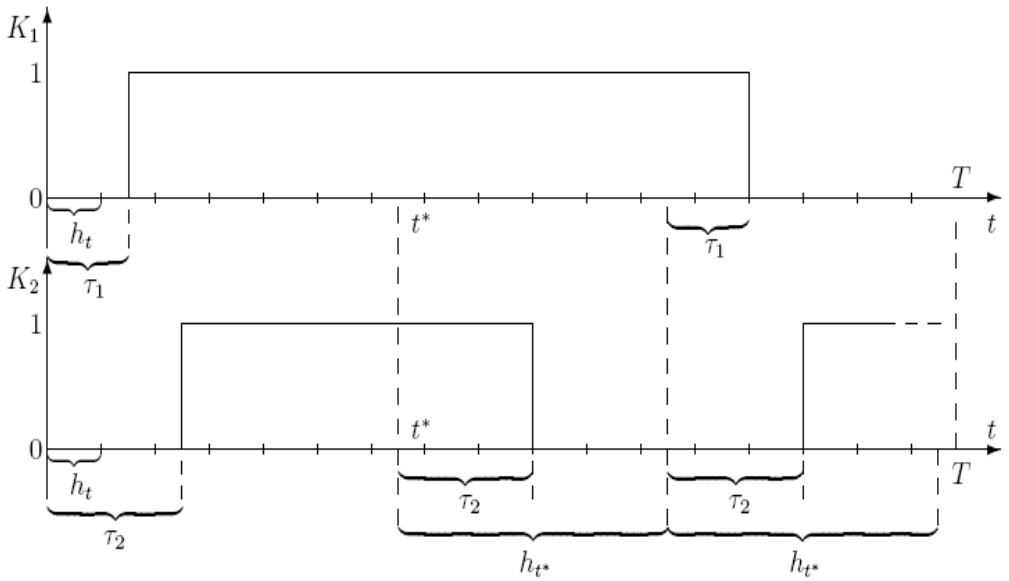


Figure 3.20. Time diagram of formation of values of weight coefficients.

For clearness of the work of the considered block in Figure 3.20 is given the time diagram of formation of values of weight coefficients k_i for a simple example when pollution sources are two, and both either drop given quantities of pollutants or do not drop. The drop of pollutants they begin at once at start up the manufacture. After certain time t^*, the second pollution source damages, i.e. it stops dropping pollutants, and over $t^* + h_{t^*}$, the first pollution source damages, at the same time the second pollution source begins operation, i.e. it drops the pollutants. The intervals τ_1 and τ_2 are times of water running from the first and the second pollution sources up to controled point, respectively.

In a case, showed in Figure 3.21, the mathematical models of recalculation of pollutants concentrations look like

$$
\begin{aligned}
&q(t)=\sum_{i=1}^{5} K_i q_i(t);\; A(t)=\frac{1}{q(t)}\sum_{i=1}^{5} k_i a_i(t-\tau_i)q_i(t-\tau_1)+C_1x_1(t);\\
&B(t)=\frac{1}{q(t)}\sum_{i=1}^{5} k_i b_{i-2}(t-\tau_i)q_i(t-\tau_i)+C_2x_2(t);\\
&C(t)=\frac{1}{q(t)}\left[k_5 C(t-\tau_5)q_5(t-\tau_5)\right]+C_3x_3(t);\; D(t)=\frac{1}{q(t)}\left[k_5 d(t-\tau_5)q_5(t-\tau_5)\right]+C_3x_4(t);\\
&E(t)=\frac{1}{q(t)}\left[k_5 l(t-\tau_5)q_5(t-\tau_5)\right]+C_3x_5(t);
\end{aligned}
\qquad (3.38)
$$

where

$$C_1 = \begin{cases} 1 \ \ at \ \ \ k_1 \neq 0 \vee k_2 \neq 0 \vee k_3 \neq 0 \vee k_4 \neq 0 \vee k_5 \neq 0, \\ 0 - \text{otherwise}, \end{cases}$$

$$C_2 = \begin{cases} 1 \ \ at \ \ \ k_3 \neq 0 \vee k_4 \neq 0 \vee k_5 \neq 0, \\ 0 - \text{otherwise}, \end{cases}$$

$$C_3 = \begin{cases} 1 \ \ at \ \ \ k_5 \neq 0, \\ 0 - \text{otherwise}. \end{cases}$$

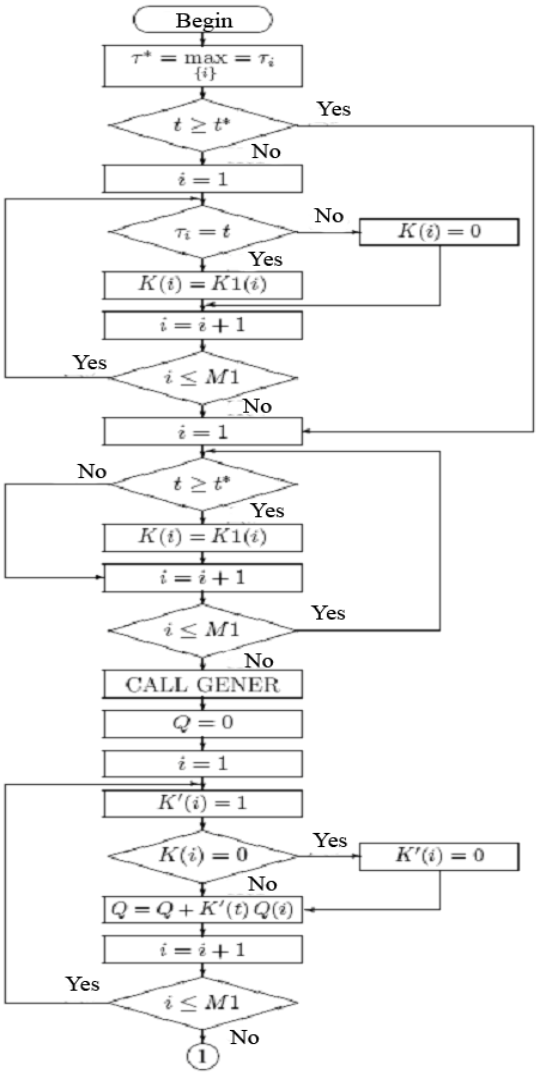


Figure 3.21 (Continued).

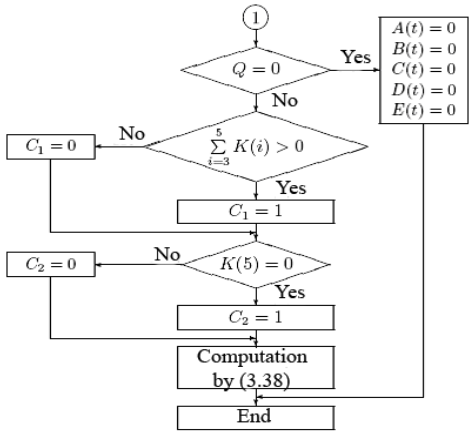


Figure 3.21. The bookkeeping scheme of the algorithm of simulation of pollutants concentrations.

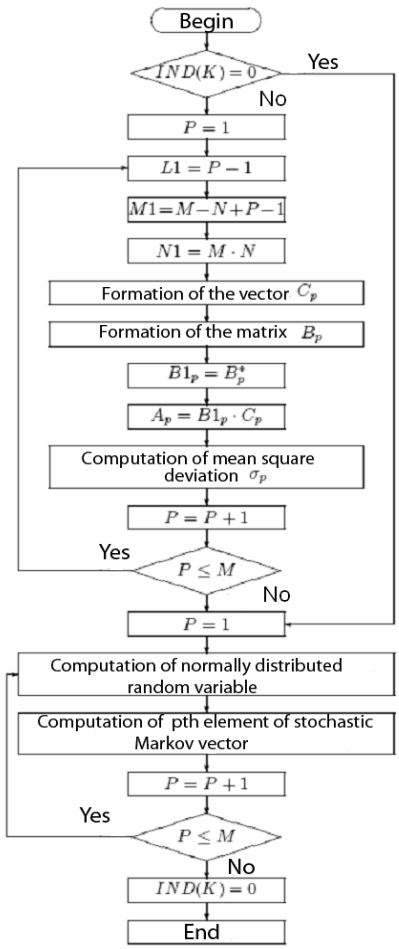


Figure 3.22. The bookkeeping scheme of the algorithm of simulation of multi-dimensional normal Markov process with given depth of connectivity.

The result of the work of the block, reduced in Figure 3.22, for one unit of time pass, are elements of M -dimentional random vector $X_p, p = 1,...,M$. For their definition, the coefficients b_ℓ^p, $\ell = 1, p = 1$; $a_{i,j}^p$, $i = 1,...,M$, $j = 1,...,N$; $\sigma_p, p = 1,...,M$, with the help of auto- and intercovariation functions, are calculated. Because of the stochastic component of the concentration of pollutants is quasi-stationary, the values of auto- and intercovariation functions are necessary to re-calculate periodically. Accordingly, it is necessary to re-calculate unknown coefficients, and during stationarity of the process, it is necessary to use their earlier calculated values. With this purpose the elements of the set IND are used, which take on two values (0 or 1) depending on the necessity of recalculation of unknown coefficients. Normally distributed random numbers are used in simulation, which are calculated by simple transformation of standard, uniformly distributed random numbers generated by standard generator of pseudo-random numbers (see Appendix 1, 2, 3).

The developed simulation models were used for generating measured values of controled parameters of sewages of the factory. On the basis of this information, the software of the automated quality monitoring system of these waters was tested and optimized [1, 118, 119].

3.7. Simulation of Real Multidimensional Stationary Gauss-Markov Series with Given Depth of Connectivity

As a rule, the stochastic component of the process of formation of the condition of the environment approximates by Gauss-Markov series due to its limiting properties [83, 117, 120]. The exhausting information about Markov processes are adduced in the works [121-123]. As the objects of the environment are multydimensional with statistically inter-related parameters, we shall bound by consideration of the simulation of multidimensional Markov series. One-dimensional Markov series are their particular case.

The simulation of multidimensional random series by computers is widely used at solving many applied problems. The methods of group simulation of inter-correlated time series are considered in the works [122, 124-125]. The methods of simulation of multidimensional Gauss-Markov series with single depth of connectivity is offered in [125, 126]. The problem of not equidistantness of the simulated results is automatically solved in it; the problem of selection of initial conditions becomes almost trivial, it excludes the transition process and the possibility of using of all elements of the simulated sequence. The method of the autoregression with integrated moving average (MAIMA) is described in the work [124]. The limitedness of the method is the following: it supposes the identity of conditional and unconditional distributions of the random series. Except for the described methods, in [122] is adduced the more general linear regression method at simulation of equidistant realization of multidimensional Gauss-Markov series. Its advantage is also in sufficient simplicity and convenience of realization of this method by comparison with other methods.

All these methods of simulation of random series imply the availability of certain a prior information: multidimensional distribution function or spectral density, the vector of mathematical expectations and covariance function and so on, which one, as a rule, is given as observation results, by which the unknown characteristics of random series estimate. The errors made in estimations influence the accuracy of simulation results.

Let us consider the dependence of the accuracy of simulation on the errors of estimation of characteristics of modelled series [127]. The stationary Gauss-Markov series is completely determined by giving of the covariance matrix. Therefore m-dimensional Gauss-Markov series $X(t)=(x_1(t),x_2(t),...,x_m(t))$ with depth of connectivity equal to N can be presented as [122, 126]

$$x_p(t)=\sum_{\ell=1}^{p-1} b_\ell^p x_\ell(t)+\sum_{i=1}^{m}\sum_{j=1}^{N} a_{ij}^p x_i(t-j)+\sigma_p\xi_p(t), \tag{3.39}$$

where b_ℓ^p, a_{ij}^p are the coefficients dependent on the auto- and inter-covariation functions of m-dimensional random series $X(t)=(x_1(t),x_2(t),...,x_m(m))$; σ_p^2 is the residual variance of the random series $x_p(t)$; $\xi_p(t)$ is standard normally distributed random variable.

The unknown coefficients and the residual variance in (3.39) are determined by the method of least squares. Using the designations

$$R'_{k,i}\left(\left|h-j\right|\right)=\begin{cases} R_{k,i}\left(\left|h-j\right|\right) \;\; at \;\; h\geq j, \\ R_{i,k}\left(\left|h-j\right|\right) \;\; at \;\; h<j, \end{cases}$$

$$k,i=1,...,m;\;\; j,n=1,...,N;$$

$$A_p^T=\left(b^p,a^p\right)_{1\times[mN+(p-1)]};\;\; C_p^T=\left(R_{k,i}\left(h\right)\right)_{1\times mN};$$

$$B_p=\left(R'_{k,i}\left(\left|h-j\right|\right)\right)_{mN\times[mN+(p-1)]},\;\; p=1,...,m,$$

where $R_{k,i}\left(\left|h-j\right|\right)$ are the suitable covariations, the expression for unknown coefficients becomes

$$A_p=B_p^+C_p, \tag{3.40}$$

where B_p^+ is the pseudoinverse matrix [128, 129]; the expression for the residual variance is

$$\begin{aligned}\sigma_p^2=R_p(0)-\sum_{\ell=1}^{p-1}\sum_{k=1}^{p-1} b_\ell^p b_k^p R_{i,k}(0)-\sum_{i=1}^{m}\sum_{j=1}^{N}\sum_{k=1}^{m}\sum_{\ell=1}^{N} a_{k\ell}^p a_{ij}^p R'_{i,k}\left(\left|\ell-j\right|\right)- \\ -2\sum_{\ell=1}^{p-1}\sum_{j=1}^{N}\sum_{i=1}^{m} b_\ell^p a_{ij}^p R_{i,\ell}(j),\end{aligned} \tag{3.41}$$

where $R_p(0)$ is the variance of p th stochastic process.

Let us estimate the error of simulation. First of all, it depends on the accuracy of estimations of the values of covariance functions of the natural data and, also, from the accuracy of the solution of the system of linear equations (3.40). Let us designate

$$X_p^T(t-1)=\left(x_1(t),x_2(t),...,x_{p-1}(t),x_1(t-1),x_1(t-2),...,x_1(t-N),x_2(t-1),...,x_m(t-N)\right),$$
$$p=1,...,m.$$

The sizes of the column vector $X_p(t-1)$ are equal to $\left[m\cdot N+(p-1)\right]\times 1$. Let us rewrite (3.39) as follows:

$$x_p(t)=A_p^T X_p(t-1)+\sigma_p\xi_p(t),\ \ p=1,...,m, \tag{3.42}$$

where A_p is determined by the expression (3.40).

Elements of the matrices B_p and C_p are the values of the auto- and inter covariation functions computed by experimental data. Therefore, in a real case, not exact values of matrices B_p and C_p, but their estimations $\hat{B}_p$ and $\hat{C}_p$ are known. Let us designate $\hat{B}_p=B_p+\xi_p$, $\hat{C}_p=C_p+\varepsilon_p$, where ξ_p and ε_p are the matrices of calculation errors of the matrices B_p and C_p, respectively.

Thus, in a real case, for the determination of A_p we have the system of equations

$$\hat{B}_p A_p=\hat{C}_p. \tag{3.43}$$

Let us designate by $\hat{A}_{p0}$ the normal pseudo-solution of the system (3.43). Then $\hat{A}_{p0}=\hat{B}_p+\hat{C}_p$ and there takes place $\hat{A}_{p0}=A_{p0}+\Delta A_{p0}$, where ΔA_{p0} is the absolute error of calculation of the matrix A_{p0}. Let us introduce the following designations also

$$\delta A_{p0}=\frac{\left\|\hat{A}_{p0}-A_{p0}\right\|}{\left\|A_{p0}\right\|},\ \ \delta B_p=\frac{\left\|\xi_p\right\|}{\left\|B_p\right\|},\ \ \delta C_p=\frac{\left\|\varepsilon_p\right\|}{\left\|C_p\right\|},$$

where $\|\cdot\|$ is the Euclidean norm of the suitable matrix. Let us suppose that δB_p and δC_p are quite small values. Then, in accordance with [129] the following estimation is valid

$$\delta A_{p0}\le cond^+ B_p\left(\delta B_p+\delta C_p\right), \tag{3.44}$$

where $cond^+ B_p=\left\|B_p\right\|\cdot\left\|B_p^+\right\|$ is the condition number of the matrix B_p.

The use of the estimation $\hat{A}_{p0}$ in (3.42) results in errors of simulation, i.e. in reality the following random series is modeled

$$\hat{x}_p(t) = \hat{A}_{p0}^T X_p(t-1) + \hat{\sigma}_p \xi_p(t), \qquad p = 1,...,m, \tag{3.45}$$

where $\hat{\sigma}_p = \sigma_p + \Delta\sigma_p$, $\Delta\sigma_p$ is the absolute error of calculation of the residual of the standard deviation σ_p.

Let us suppose that the exact values of the initial vectors $X_1(t-1),...,X_1(t-N)$, $X_2(t-1),...,X_m(t-N)$ are known, and also the residual standard deviations $\sigma_p, p = 1,...,m,$ of the modelled process are known. We shall rewrite (3.45) by the way

$$\hat{x}_p(t) = (A_{p0}^T + \Delta A_{p0}^T)\, X_p(t-1) + \sigma_p\, \xi_p(t), \quad p = 1,...,m, \tag{3.46}$$

The recurrent formula of definition of the generated random series on k th step looks like

$$\hat{x}_p(t+k) = \left(A_{p0}^T + \Delta A_{p0}^T\right)\left(X_p(t+k-1) + \Delta X_p(t+k-1)\right) + \\ + \sigma_p\, \xi_p(t+k),$$

where $X_p(t+k-1)$ is the vector of exact values of generated series on $(t+k-1)$ th step; $\Delta X_p(t+k-1)$ is the vector of absolute errors on $(k-1)$th step computed values of the generated series

$$\Delta X_p^T(t+k-1) = (\Delta X_1(t+k-1) X_1(t+k-2),...$$
$$...,\sum_{i=1}^{p-1} \Delta X_i(t+k-1) X_i(t+k-2), \Delta A_1^T X_1(t+k-2),$$
$$\Delta A_1^T X_1(t+k-3),...,\Delta A_1^T X_1(t+k-N-1),$$
$$\Delta A_2^T X_2(t+k-2),...,\Delta A_2^T X_2(t+k-N-1),...,$$
$$\Delta A_m^T X_m(t+k-2),...,\Delta A_m^T X_m(t+k-N-1))_{1\times[mN+(p-1)]}.$$

The absolute error of computed value of the generated series (3.46) is

$$\left|\Delta x_p(t+k)\right| = \left\| A_{p0}^T\, \Delta X_p(t+k-1) + \Delta A_{p0}^T\, \hat{X}_p(t+k-1) \right\|, \tag{3.47}$$

where $\hat{X}_p(t+k-1)$ is computed values of the generated series on $(t+k-1)$ th step.

Let us determine the condition to which should to satisfy the error of calculation of estimations of the elements of inter-covariation matrix of the generated series, so that for any $k \geq 1$ there was fulfilled

$$P\left(\left|\Delta x_p(t+k)\right| \leq \gamma_p\right) \geq 1-\alpha, \quad \forall p:\ p \in (1,...,m). \tag{3.48}$$

To take into account (3.43), (3.46), we have

$$P\left(\left|\Delta x_p(t+k)\right| \le \gamma\right) \ge P(\left\|A_{p0}^T\right\|\left\|\Delta X_p(t+k-1)\right\| +$$
$$+ \left\|A_{p0}^T\right\|\left\|\widehat{X}_p(t+k-1)\right\| \le \gamma) \ge P(\left\|A_{p0}\right\|(\left\|\Delta X_p(t+k-1)\right\| +$$
$$+ cond^+ B_p(\delta B_p + \delta C_p)\left\|\widehat{X}_p(t+k-1)\right\|) \le \gamma).$$

Therefore, if γ is determined from the condition

$$P(\left\|A_{p0}\right\|(\left\|\Delta X_p(t+k-1)\right\| + cond^+ B_p(\delta B_p + \delta C_p)\left\|\widehat{X}_p(t+k-1)\right\|) \le \gamma) = 1-\alpha, \tag{3.49}$$

then (3.48) takes place.

Let us consider the case, when in the model (3.39) are left out the current values of modelled series, i.e. when $b_\ell^p = 0, \quad \ell = 1,...,p-1, \quad p = 1,...,m$. At this time, the matrix B_p is quadratic.

The random variable $\widehat{X}_p(i-j)$ is obeyed the normal distribution law with mathematical expectation equal to 0, and variance $R_p(0)$. Therefore it is always possible to find the value β_p for which there takes place

$$P\left(\left|\widehat{x}_p(t-j)\right| \le \beta_p\right) = 1-\alpha.$$

Taking into account the property of reproducibility of χ^2-probability distributions, we write

$$P\left(\left\|\widehat{X}_p(t+k-1)\right\| \le D\right) = P\left\{\left(\sum_{i=1}^{m}\sum_{j=1}^{N}\left|\widehat{x}_i(t-j)\right|^2\right)^{1/2} \le D\right\} \ge 1-\alpha, \tag{3.50}$$

where $D = N^{1/2}\left(\sum_{i=1}^{m}\beta_i^2\right)^{1/2}$. For estimation of the norm of the vector of errors we analogously obtain

$$P\left(\left\|\Delta X_p(t+k-1)\right\| \le d\right) = P\left\{\left(\sum_{i=1}^{m}\sum_{j=1}^{N}\left|\Delta A_i^T X_i(t-j)\right|^2\right)^{1/2} \le d\right\} \ge 1-\alpha, \tag{3.51}$$

where

$$d = N^{1/2}\left(\sum_{i=1}^{m}\beta_i^2\right)^{1/2}\left[\sum_{i=1}^{m}\left(cond^{+}B_i\left\|A_{i0}\right\|(\delta B_i+\delta C_i)\right)^2\right]^{1/2}.$$

By taking into account (3.50), (3.51), the ratio (3.49) can be rewritten as follows:

$$P\{\left\|A_{p0}\right\|(\left\|\Delta X_p(t+k-1)\right\|+cond^{+}B_p(\delta B_p+\delta C_p)\left\|\hat{X}_p(t+k-1)\right\|)\le$$
$$\le\left\|A_{p0}\right\|\left(d+cond^{+}B_p(\delta B_p+\delta C_p)D\right)\}=1-\alpha,$$

Thus, if γ_p satisfys the condition

$$\left\|A_{p0}\right\|\left(d+cond^{+}B_p(\delta B_p+\delta C_p)D\right)\le\gamma_p, \tag{3.52}$$

then the ratio (3.48) will take place.

Let us designate the maximum absolute error of calculation of a value of the covariance function by Δ_R. Then

$$\left\|\xi_p\right\|\le\left[m^2N^2+mN(p-1)\right]^{1/2}\Delta_R,\left\|\varepsilon_p\right\|\le(mN)^{1/2}\cdot\Delta_R$$

and the ratio (3.52) will be rewritten in such a way:

$$\Delta_R\le\frac{\gamma_p}{N^{1/2}\left(\sum_{i=1}^{m}\beta_i^2\right)^{1/2}\left\|A_{p0}\right\|\left\{N^{1/2}\left[\sum_{i=1}^{m}\left(cond^{+}B_i\left\|A_{i0}\right\|D_i\right)^2\right]^{1/2}+cond^{+}B_pD_p\right\}};$$
$$D_i=\frac{\left[m^2N^2+mN(i-1)\right]^{1/2}\left\|C_i\right\|+(mN)^{1/2}\left\|B_i\right\|}{\left\|B_i\right\|\cdot\left\|C_i\right\|},\quad i=1,\ldots,m. \tag{3.53}$$

Thus, if the condition (3.53) is fulfilled for all $p=1,\ldots,m$, then the multidimensional Gauss-Markov series is generated with given accuracy by probability greater than or equal to $1-\alpha$. The sample size n, ensuring the calculation of values of the covariance function with absolute error which do not surpass Δ_R, is determined by the ratio (3.48).

Let us consider now the general case, when in the model (3.39), the current values of the modelled series are allowed. At such case, the expressions (3.50), (3.51) take the forms, respectively:

$$P\left(\left\|\widehat{X}_p(t+k-1)\right\| \le D\right) = P\left\{\left(\sum_{i=1}^{m}\sum_{j=1}^{N}\left|\widehat{x}_i(t-j)\right|^2 + \sum_{\ell=1}^{p-1}\left|\widehat{x}_\ell(t)\right|^2\right)^{1/2} \le D\right\} \ge 1-\alpha, \tag{3.54}$$

where

$$D = \left[(N+1)\sum_{i=1}^{p-1}\beta_i^2 + N\sum_{i=p}^{m}\beta_i^2\right]^{1/2};$$

$$P\left(\left\|\Delta X_p(t+k-1)\right\| \le Q_p\right) =$$

$$= P\left\{\left(\sum_{i=1}^{m}\sum_{j=1}^{N}\left|\Delta A_i^T X_i(t-j)\right|^2 + \sum_{\ell=1}^{p-1}\sum_{d=1}^{\ell}\left|\Delta X_d(t+k-1)X_d(t+k-2)\right|^2\right)^{1/2} \le Q_p\right\} \ge \tag{3.55}$$

$$\ge P\left\{\left(\sum_{i=1}^{m}\sum_{j=1}^{N}\left\|\Delta A_i^T\right\|^2\left\|X_i(t-j)\right\|^2 + \sum_{\ell=1}^{p-1}\sum_{d=1}^{\ell}\left\|\Delta X_d(t+k-1)\right\|^2\left\|X_d(t+k-2)\right\|^2\right)^{1/2} \le Q_d\right\} \ge 1-\alpha,$$

where

$$Q_1 = d; \quad Q_p = \left\{N\left(\sum_{i=1}^{m}\beta_i^2\right)\left[\sum_{i=1}^{m}\left(cond^{+}B_i\left\|A_{i0}\right\|(\delta B_i + \delta C_i)\right)^2 + \sum_{\ell=1}^{p-1}\ell Q_\ell\right]\right\}^{1/2}.$$

Thus, we have the recurrent ratio (3.55), permitting to estimate from above the random variable $\left\|\Delta X_p(t+k-1)\right\|$ with given probability for the general case of the model (3.39). It is necessary to note that the estimations (3.50), (3.51), (3.54) do not depend on the time parameter, i.e. the error of simulation of multidimensional time series is determined by the error of calculation of the matrices B_p and C_p, the elements of which are the values of covariance functions, and also by conditionality of the matrices B_p, by the norms of the vectors A_{p0}, by the residual variance σ_p^2 of the modelled series, by its dimensionality and the depth of connectivity. Therefore, before of beginning the simulation of the multidimensional series it is necessary, by the ratio (3.54), to estimate Δ_R - the error of calculation of values of covariance functions, ensuring the given error of simulation.

By taking into account the error of calculation of the residual variance of the modelled series, the absolute error of simulation (3.47) takes the form:

$$\Delta x_p(t+k) = A_{p0}^T \Delta X_p(t+k-1) + \Delta A_{p0}^T \widehat{X}_p(t+k-1) + \Delta\sigma_p \xi_p(t+k).$$

Let us write the expression (3.41) in matrix form

$$\sigma_p^2 = R_p(0) - A^T_{p_1\times[mN+(p-1)]} R_{[mN+(p-1)][mN+(p+1)]} A_{p_{[mN+(p-1)]\times 1}} - 2B1^T_{p_1\times(p-1)} R1_{(p-1)\times 1}, \tag{3.56}$$

where

$$B1_p = \left(b^p\right)_{(p-1)\times 1}; R1^T = \left(R1(1),..., R1(p-1)\right);$$

$$R1(\ell) = \left(A1_{1\times mN} R(\ell)_{mN\times 1}\right);\ \ \ell = 1,..., p-1;\ \ A1_p^T = \left(a^p\right)_{1\times mN}.$$

By taking into account the errors, the expression (3.56) can be rewritten as follows:

$$\sigma_p^2 + \Delta\sigma_p^2 = R_p(0) + \Delta R_p(0) - (A_p^T + \Delta A_p^T)(R + \Delta R)(A_p + A) -$$
$$- 2(B1_p^T + \Delta B1_p^T)(R1_p + \Delta R1_p).$$

From here, for the error of calculation of the residual variance, we obtain the ratio

$$\begin{aligned}\left|\Delta\sigma_p\right|^2 \le{}& \left|\Delta R_p(0)\right| + 2\left\|A_p^T\right\|\cdot\|R\|\cdot\left\|\Delta A_p\right\| + \left\|\Delta A_p^T\right\|\cdot\|\Delta R\|\cdot\left\|A_p\right\| + \\ &+ \left\|\Delta A_p^T\right\|\cdot\|R\|\cdot\left\|\Delta A_p\right\| + \left\|\Delta A_p^T\right\|\cdot\|\Delta R\|\cdot\left\|\Delta A_p\right\| + \\ &+ 2\left(\left\|R1_p^T\right\|\cdot\left\|\Delta R1_p\right\| + \left\|\Delta B1_p^T\right\|\cdot\left\|R1_p\right\| + \left\|\Delta B1_p^T\right\|\cdot\left\|\Delta R1_p\right\|\right).\end{aligned} \tag{3.57}$$

At fulfilling the condition (3.53), the error of calculation of the variance (3.57) will be insignificant. If in (3.57) to neglect the additives of higher order, then for estimation of the error of the residual variance of modelled process, it is fair

$$\left|\Delta\sigma_p\right|^2 \le \Delta_R + 2\left(\left\|A_p^T\right\|\cdot\|R\|\cdot\left\|\Delta A_p\right\| + \left\|B1_p^T\right\|\cdot\left\|\Delta R1_p\right\| + \left\|\Delta B1_p^T\right\|\cdot\left\|R1_p\right\|\right), \tag{3.58}$$

where

$$\left\|\Delta R1_p\right\| = \left(\sum_{\ell=1}^{p-1}\left\|\Delta R1(\ell)\right\|^2\right)^{1/2};$$

$$\left\|\Delta R1(\ell)\right\| \le \left\|\Delta A1_p\right\|\cdot\left\|R(\ell)\right\| + \left\|A1_p\right\|\cdot\left\|\Delta R(\ell)\right\| + \left\|\Delta A1_p\right\|\cdot\left\|\Delta R(\ell)\right\|;$$

$$\left\|\Delta R(\ell)\right\| \le (mN)^{1/2}\Delta_R;\quad \left\|\Delta B1_p\right\| < \left\|\Delta A_p\right\|;\quad \left\|\Delta A1_p\right\| \le \left\|\Delta A_p\right\|.$$

The error of calculation of the residual variance of the modelled series is taken into account by adding the estimation from above of $\Delta\sigma_p$ in the left-hand part of the expression (3.52), calculated by the ratio (3.58).

The reduced results are obtained in the supposition that the system of linear equations

$$B_p A_p = C_p \tag{3.59}$$

is compatible. The compatibility of the system (3.59) means that

$$B_p^+ B_p - E = 0, \tag{3.60}$$

where E is the unit matrix.

The algorithm of calculation of B_p^+ has an error, therefore the condition (3.60) will be fulfilled with certain error. Let us designate by ΔB_p^+ the error of calculation of B_p^+, i.e. $\widehat{B}_p^+ = B_p^+ + \Delta B_p^+$. The system (3.58) is compatible, if

$$0 \le \left\| \widehat{B}_p^+ B_p - E \right\| \le \left\| B_p \right\| \left\| \Delta B_p^+ \right\|.$$

The noncompatibility of (3.59) means that $M(x_p(t)) \ne A_p^T M(X_p(t-1))$, i.e. even at $M(X_p(t-1)) = 0$ there takes place $M(x_p(t)) \ne 0$. Because of this reason, the value $M(x_p(t+k))(k>0)$ moreover will not be equal to zero. The mathematical expectation of $x_p(t)$ will incrase the faster, the biger the elements of the vector A_p are, i.e. the biger the modulus of the vector A_p is. If all the elements of the vector A_p are less than unit, then by increasing k, $M(x_p(t+k))$ will tend to zero, i.e. the modelled random series in time will be stable. Otherwise the series will be divergent. The variance of the series will behave analogously. The modelled series will be divergent, if given covariance functions are also divergent. The negativity of the calculated value of the variance by the ratio (3.41) means that Gauss-Markov series with given characteristics can not be modelled by the model (3.39).

Example. For checking the condition (3.53) there were simulated 2100 realizations of onedimensional Gauss-Markov series by (3.39) with the following auto-correlation function: $R(0)=1;\quad R(0)=1;\quad R(1)=0.2457;\quad R(2)=0.3235;\quad R(3)=0.138;\quad R(4)=0.0516;$ $R(5)=0.0488;\quad R(6)=0.00157;\quad R(7)=-0.00233$, i.e. $m=1,\ N=7$. In this case: $\left\|B^+B-E\right\| = 0.153105\cdot 10^{-4}$; $\|C\| = 0.434875$; $\|B\| = 2.99145$; $\|A\| = 0.0519399$; $\left\|B^+\right\| = 4.603693$ and $cond^+ B = 13.77171$. The ratio (3.53) takes the form $\Delta_R \le 0.0183825\cdot\gamma$. By the simulated values of the series there were computed the estimations of the auto-correlation function: $\widehat{R}(0) = 0.965998;\quad \widehat{R}(1) = 0.256597;\quad \widehat{R}(2) = 0.322361;\quad \widehat{R}(3) = 0.108244;$ $\widehat{R}(4) = 0.0585888;\quad \widehat{R}(5) = 0.573747;\quad \widehat{R}(6) = 0.00858013;\quad \widehat{R}(7) = 0.0053352.$ In accordance with (3.48), the error of computed estimations does not exceed $\Delta_R = 0.039$ with given probability, in which we are convinced by direct comparison of the given and computed estimations of values of the auto-correlation function. By the model (3.39) were modelled 2100 realizations of onedimensional Markov series with estimated values of the auto-correlation function. At simulation were used the same independent, normally distributed pseudo-random values, which were used at simulation with given values of auto-correlation function. The comparison of the suitable values of the simulated series, obtained in both cases, has shown the justice of the ratio (3.48), which takes the form $\left|\widehat{x}(t) - x(t)\right| \le 0.471346$ with probability greater than 0.95.

Chapter 4

METHODS OF MAKING DECISIONS IN MONITORING OF RIVER POLLUTION

One of the basic sections of stochastic mathematics is the theory of decision making [132]. The given chapter is dedicated to problems of elaboration of new methods of making decisions in the systems of monitoring and control of pollution of objects of the environment. In particular, it is dedicated to the problem of acceptance of statistical hypothesis by results of experiment, founded on one of the classical approaches - the Bayesian approach [133].

Mathematical base of making decisions in recognition problems is the theory of games and, particularly, one of its concrete branch – the theory of statistical decisions, which one can be interpreted as the theory of acceptance of the optimum decisions on the basis of trials.

The basic results of the theory of the statistical decisions were obtained by Wald [134, 135]. Detailed study of the fundamentals of this theory is contained in the monography of Blackwell and Girshick [136], in the work of Lehmann [137]. The special attention is given to Bayesian criterion in the works of Wald, Blackwell and Girshick. Complete theory of statistical decisions is factual contained in these monographies. Fundamental aspects of classical theory are set forth in monographies of Wilks [138], Rao [139], Kendall and Stuart [102], De Groot [140], Cramer [141], Zacks [142], Aivazjan, Yenyukov and Meshalkin [143] etc.

There are different classical criterions of testing hypotheses depending on selected criterion [102, 136-142, 144-149]: the Fisher's criterion, the criterion of Neyman-Pearson, sequential criterion of Wald, Bayesian criterion, maximum of posterior probabilities, maximum likelihood criterion, mini-max test etc. A lot of works in theoretical and applied statistics are dedicated to the synthesis of optimum rules of making the decisions [146, 148–165, 166–175 etc.]. However, in despite of variety of the works dedicated to the problem of statistical hypotheses test and, in particular, to Bayesian test, no one of these works do not consider Bayesian problem of many hypotheses testing from such point of view as in the works of the authors [1, 133, 176-182]. Some results of the author from these works are generalized in this chapter and a number of more perfect algorithms of their solution are designed. For the first time there are entered two loss functions allowing to pass from an unconditional optimization problem to a conditional problem which one allows by imposing of restrictions on probabilities of errors of the first and second kind to introduce a loss function indirectly when a priori it is difficultly to make [133, 183].

4.1. GENERALIZATION OF BAYESIAN RULE OF MANY HYPOTHESES TESTING

The essence of the problem of statistical hypotheses testing may be formalized in the following way [133]. Let us consider n independent identically distributed random quantities $x_1,...,x_n$, which have joint probability distribution density $p(x,a) = p(x_1,...,x_n;a_1,...,a_k)$, given on σ-algebra of Borellian sets of space $R^n (x \in R^n)$ which is called a sample space, while $\theta^k (a \in \theta^k)$-a parameter space. Assume that form of function $p(x,a)$ is known, and parameters a must be estimated on the basis of experiment x results. The assumption that parameter a belongs to set $A_i \in \theta^k, i = 1,...,S$ is called "a statistical hypothesis" and is denoted by letter H_i. If set A_i consists of only one point, the hypothesis is simple, otherwise H_i is a composite hypothesis. Hypothesis testing problem consists in accepting of one hypothesis out of the given set of hypotheses $\{H_1, H_2,..., H_S\}$ on the basis of experimental results, so as to minimize the criterion defining the error probability.

There are different methods of statistical hypotheses testing [102, 133, 137, 142]. Among them, the Bayesian approach has a special place. A generalization of Bayesian rule of many hypotheses testing is given below. It consists in increasing of decision rule dimensionality with respect to the number of tested hypotheses, which allows one to make decisions more differentially than in the classical case and to state, instead of unconditional optimization problem, conditional one that enables to make guaranteed decisions concerning errors of true decisions rejection, which is the key point when solving a number of practical problems. These generalizations are given both for a set of simple hypotheses, each containing one space point, and hypotheses containing a finite set of separated space points.

Generally, when the hypotheses contain some spatial points and thus one and those points can enter into different hypotheses, the task of testing multiple hypotheses on a basis of the Bayesian approach looks as follows.

Let $x' = (x'_1,...,x'_n)$ be independent identically distributed random quantities that have joint probability distribution function $F(x' \mid a')$ given on σ-algebra of Borellian sets of space $R^n, a' \in \Theta$, where Θ is n-dimensional parametric space[1]. Let $\{a'_1,...,a'_N\}$ be the finite number of given values of parameter a'. It is known, that $M (M \le N)$ parameters out of set $\{a'_1,...,a'_N\}$ are true. It is necessary to separate values of these true parameters.

[1] The assumption of independence at normal probability distribution is not a rigid restriction, as by linear transformation of the vector of correlated normal random quantities, it is not difficult to obtain the vector of non-correlated random quantities. Performing of preliminary decorrelation does not affect hypotheses testing results, so called "information discrepancy of hypotheses" does not change in case of non-degenerate transformation [184].

Let $H_1,...,H_S$, $S \le C_N^M$, be a set of hypotheses concerning truth of parameters a. Hypothesis H_i supposes that i th combination of M parameters a', $H_i = \{a'_{i_1},..., a'_{i_M}\}$ is true. In general case, hypotheses H_i, $i = 1,...,S$, intersect, i.e. contain common parameters. Let us denote: $x = (x'_1,..., x'_M) \equiv (x_1,..., x_m)$, $a^i = (a'_{i_1},..., a'_{i_M}) \equiv (a^i_1,..., a^i_m)$, where $m = n \cdot M$; $p(H_i)$-*a priori* probability of hypothesis H_i; $p(x \mid H_i)$-probability distribution density of x at truth of hypothesis H_i; $D = \{d\}$-a set of solutions, where $d = \{d_1,..., d_N\}$, it being so that

$$d_j = \begin{cases} 1, \text{ if the decision that parameter } a'_j \text{ is true is made,} \\ 0, \text{ otherwise;} \end{cases}$$

$\delta(x) = \{\delta_1(x),..., \delta_N(x)\}$-the decision function that associates each measurement vector x with a certain decision

$$x \xrightarrow{\delta(\cdot)} d \in D;$$

$\Gamma_j = \{x : \delta_j(x) = 1\}$, i.e. Γ_j is the set of those x, for which the decision on truth of parameter a_j is made, $\Gamma_j \in X$, where $X - m$-dimensional measurement space. It is obvious that $\delta(x)$ is completely determined by the Γ_j regions, i.e. $\delta(x) = \{\Gamma_1, \Gamma_2,..., \Gamma_N\}$.

Let hypothesis H_i be true. Let us introduce loss function $L(H_i, \delta(x))$. Then the risk corresponding to hypothesis H_i has the following form [133, 142]:

$$\rho(H_i, \delta) = \int_X L(H_i, \delta(x))\, p(x \mid H_i) dx.$$

For each decision rule $\delta(x)$, risk function

$$R(\delta) = \sum_{i=1}^{S} \rho(H_i, \delta)\, p(H_i) = \sum_{i=1}^{S} p(H_i) \int_X L(H_i, \delta(x))\, p(x \mid H_i) dx. \quad (4.1)$$

The problem consists in finding of such decision rule $\delta^*(x)$, i.e. in finding of such Γ_j, $j = 1,..., N$, regions of parameters a_j acceptance, for which the following will hold

$$R\left(\delta^*\right)=\min_{\{\delta\}} R\left(\delta\right). \tag{4.2}$$

4.2. General Solutions of Unconditional and Conditional Bayesian Tasks

The presented statement is generalization of the classical Bayesian problem of many simple hypotheses testing, as the latter is obtained from the above-described statement, when the number of points in hypothesis H_i, $M=1$. Besides, unlike the classical statement, where dimensionality of decision function is equal to the number of tested hypotheses, in this statement the decision is made more differentially regarding not the hypotheses as a whole, but parameters that form these hypotheses. Therefore, decision rule dimensionality N exceeds the number of hypotheses S. This enables to impose restrictions on probabilities of falsely made decisions in more flexible way.

Let us consider the case, when none of the hypotheses pairs contain common points. The set of hypotheses in this case is: $H_1 \equiv \left\{a'_1,..,a'_M\right\},...,H_S \equiv \left\{a'_{N-M+1},...,a'_N\right\}$. It is obvious, that $N=M\cdot S$.

Risk function (4.1) assumes the following form [133]:

$$R\left(\delta\right)=\sum_{j=1}^{S}\sum_{i=1,i\neq j}^{S} L(H_i,H_j)p(H_i)\int_{E_j} p(x\,|\,H_i)dx, \tag{4.3}$$

where E_j-hypothesis H_j acceptance region. It is clear that $\Gamma_1=...=\Gamma_M=E_1$, $\Gamma_{M+1}=...=\Gamma_{2M}=E_2,\ ...,\ \Gamma_{N-M+1}=...=\Gamma_N=E_S$.

At $M=1$ problem (4.3) comes to the classical Bayesian problem of many simple hypotheses testing.

In general case, loss function $L(H_i,\delta(x))$ consists of two components

$$L\left(H_i,\delta(x)\right)=\sum_{j:a_j\notin H_i} L(H_i,\delta_j(x)=1)+\sum_{j:a_j\in H_i} L(H_i,\delta_j(x)=0), \tag{4.4}$$

i.e. loss function $L\left(H_i,\delta(x)\right)$-is the total loss due to erroneously accepted or rejected parameters a_j, at truth of hypothesis H_i.

Subject to (4.4), loss function (4.1) may be rewritten as

$$R(\delta)=\sum_{j=1}^{N}\{\int_{\Gamma_j}[\sum_{i:H_i\bar{\ni}a_j} L\left(H_1,\delta_j(x)=1\right)\, p(H_i)\, p(x\,|\,H_i)-$$
$$-\sum_{i:H_i\ni a_j} L\left(H_i,\delta_j(x)=0\right)\, p(H_i)\, p(x\,|\,H_i)]\, dx+\sum_{i:H_i\ni a_j} L\left(H_i,\delta_j(x)=0\right)\cdot p(H_i)\}. \tag{4.5}$$

It is obvious, that minimum in (4.5) is reached in the following regions of parameters a_j acceptance

$$\Gamma_j=\{x:\sum_{i:H_i\bar{\ni}a_j} L\left(H_i,\delta_j(x)=1\right)\, p(H_i)\, p(x\,|\,H_i)<$$
$$<\sum_{i:H_i\ni a_j} L\left(H_i,\delta_j(x)=0\right)\, p(H_i)\, p(x\,|\,H_i)\},\quad j=1,...,N. \tag{4.6}$$

The hypothesis H_j acceptance optimal region E_j, that minimizes the risk function (4.3), is of the following form [133, 144]:

$$E_j=\{x:\sum_{i=1}^{S}L(H_i,H_j)\, p(H_i)\, p(x\,|\,H_i)<\sum_{i=1}^{S}L(H_i,H_k)\, p(H_i)\, p(x\,|\,H_i);$$
$$\forall k:k\in(1,...,j-1,j+1,...,S)\},\quad j=1,...,S. \tag{4.7}$$

When solving diverse practical problems, either correct definition of loss function $L\left(H_i,\delta(x)\right)$ is difficult or, according to special character of a problem, a guaranteed decision with respect to errors of the first or the second kinds is required, e.g. a guarantee is required that the probability of true decision omitting error would not exceed a prescribed level. The classical Bayesian statement does not allow do that, as in it, by solution of unconditional optimization problem the total of errors of the first and the second kinds is minimized. Let us turn to the conditional optimization problem.

Let $n_f(H_i,\delta)$ and $n_{tr}(H_i,\delta)$ denote mathematical expectations of losses due to, correspondingly, falsely accepted parameters and falsely rejected parameters. Then

$$n_f(H_i,\delta)=E_x\left[\sum_{j:a_j\bar{\in}H_i}\delta_j(x)\right]=\sum_{j:a_j\bar{\in}H_i}\int_{\Gamma_j}p(x\,|\,H_i)dx,$$
$$n_{tr}(H_i,\delta)=E_x\left[\sum_{j:a_j\in H_i}(1-\delta_j(x))\right]=M-\sum_{j:a_j\in H_i}\int_{\Gamma_j}p(x\,|\,H_i)dx.$$

The mean number of false point r_δ given by rule δ is found in the following way

$$r_\delta = \sum_{i=1}^{S} p(H_i) n_f(H_i, \delta) = \sum_{i=1}^{S} p(H_i) \sum_{j: a_j \bar{\in} H_i} \int_{\Gamma_j} p(x \mid H_i) dx . \quad (4.8)$$

When considering hypotheses containing one point each, expression (4.8), i.e. the mean number of false decisions, assumes the following form

$$r_\delta = \sum_{i=1}^{S} p(H_i) \sum_{j=1, j\neq i}^{S} \int_{E_j} p(x \mid H_i) dx . \quad (4.9)$$

In order to minimize r_δ by the choice of δ, we shall require that the probability of omitting true points would not exceed a prescribed level. Let us consider possible restrictions imposed on this probability.

4.2.1. Restrictions on Conditional Probabilities of Omitting True Parameters

It is required to minimize (4.8) so that the mean share of omitted true points will not exceed prescribed level α, at truth of any of hypotheses $H_1, ..., H_S$, i.e.

$$p_{tr}(H_i, \delta) = n_{tr}(H_i, \delta)/M = 1 - \frac{1}{M} \sum_{j: a_j \in H_i} \int_{\Gamma_j} p(x \mid H_i)\, dx \le \alpha, \;\; i = 1, ..., S \quad , \quad (4.10)$$

M is the number of points corresponding of hypothesis H_i. When hypotheses H_i are simple, i.e. each of them contains one point restrictions (4.10) assume the following form

$$\int_{E_i} p(x \mid H_i)\, dx \ge 1 - \alpha, \;\; i = 1, ..., S \quad . \quad (4.11)$$

The solution of problem (4.8), (4.10) is

$$\Gamma_j = \left\{ x : \sum_{i: H_i \bar{\ni} a_j} p(H_i)\, p(x \mid H_i) < \sum_{i: H_i \ni a_j} \lambda_i \cdot p(x \mid H_i) \right\},$$

where λ_i, $i = 1, ..., S$, are defined so as to hold equality in (4.10).

The solution of problem (4.9), (4.11) is

$$E_i = \left\{ x : p(x \mid H_i) > \lambda_i \cdot \sum_{j=1, j \neq i} p(H_j)\, p(x \mid H_j) \right\}, \tag{4.12}$$

where λ_i, $i = 1, ..., S$, are defined so as to hold equality in (4.11).

4.2.2. Restrictions on Averaged Probability of Omitted True Parameters

Let us define decision rule $\delta(x)$ so as to reach the minimum in (4.8), s.t.

$$\sum_{i=1}^{S} p(H_i) p_{tr}(H_i, \delta) \leq \alpha ,$$

i.e.

$$\sum_{j=1}^{N} \int_{\Gamma_j} [\sum_{i: H_i \ni a_j} p(H_i) \cdot p(x \mid H_i)]\, dx \geq 1 - \alpha , \tag{4.13}$$

where α-the prescribed level.

For simple hypotheses, restrictions have the following form

$$\sum_{i=1}^{S} p(H_i) \cdot \int_{E_i} p(x \mid H_i)\, dx \geq 1 - \alpha . \tag{4.14}$$

The solution of problem (4.8), (4.13) is

$$\Gamma_j = \{ x : \sum_{i: H_i \bar{\ni} a_j} p(H_i) p(x \mid H_i) < \lambda \cdot \sum_{i: H_i \ni a_j} p(H_i) p(x \mid H_i) \},$$

where λ is defined so as to hold equality in (4.13).

The solution of problem (4.9), (4.14) is

$$E_j = \{ x : \sum_{i=1, i \neq j}^{S} p(H_i)\, p(x \mid H_i) < \lambda \cdot p(H_j)\, p(x \mid H_j) \}, \tag{4.15}$$

where λ, for all E_j, $j = 1, ..., S$, is one and the same scalar quantity and is defined so as to hold equality in (4.14).

4.2.3. Restrictions on Conditional Probabilities of Omitting Each True Parameter

It is required to find such decision rule $\delta(x)$ that (4.8) will be minimized, s.t.

$$\int\limits_{\Gamma_j} p(x \mid H_i)dx \geq 1-\alpha, \quad \forall j : a_j \in H_i, \quad i = 1,...,S. \tag{4.16}$$

For simple hypotheses, restrictions assume the following form

$$\int\limits_{E_i} p(x \mid H_i)dx \geq 1-\alpha, \quad i = 1,...,S. \tag{4.17}$$

The solution of problem (4.8), (4.15) is

$$\Gamma_j = \{x : \sum_{i=1}^{k_j} p(H_i)\, p(x \mid H_i) < \sum_{i=k_j+1}^{S} \lambda_{\cdot i} \cdot p(x \mid H_i)\},$$

where k_j is the number of hypotheses that don't include parameter a_j; λ_i, $i = k_j + 1,...,S$ are defined so as to hold equality in (4.16).

The solution of problem (4.9), (4.17) corresponds with (4.12).

4.2.4. Restrictions on Unconditional Probabilities of Omitting Each True Parameter

We minimize (4.8) so as to hold

$$\sum_{i:H_i \ni a_j} p(H_i \mid a_j - tr) \cdot p_{tr}(H_i, \delta_j) \leq \alpha, \tag{4.18}$$

where

$$p(H_i \mid a_j - tr) = \frac{p(a_j - tr \mid H_i) \cdot p(H_i)}{\sum\limits_{i=1}^{S} p(a_j - tr \mid H_i)\, p(H_i)},$$

$$\left(\forall i : i \in \left\{i : H_i \,\overline{\ni}\, a_j - tr\right\};\ p(a_j - tr \mid H_i) = 0\right),$$

$$\left(\forall i : i \in \left\{i : H_i \ni a_j - tr\right\};\ p(a_j - tr \mid H_i) = 1\right).$$

When hypotheses are simple, restrictions are analogous to (4.16), and solution of the problem corresponds with (4.12).

The solution of problem (4.8), (4.18) is of the following form

$$\Gamma_j = \{x : \sum_{i=1}^{k_j} p(H_i)\, p(x \mid H_i) < \lambda_j \cdot \sum_{i=k_j+1}^{S} p(x \mid H_i)\},$$

where λ_j is defined so as to hold equality in (4.18).

4.3. Algorithms of Solving Unconditional Bayesian Problems of Many Simple Hypotheses Testing

Let us introduce algorithms of implementation of hypotheses testing rules (4.6) of unconditional Bayesian problem. For simplicity of representation, let us consider the case when none hypotheses pairs has common points, i.e. the case when function of risk looks like (4.3).

Let us consider different cases of loss function $L(H_i, H_j)$ definition.

4.3.1. Step Loss Function

Let the losses due to falsely accepted hypotheses be identical, while these due to correctly made decisions be equal to zero, i.e.

$$L(H_i, H_j) = \begin{cases} C & \text{at} \quad i \neq j, \\ 0 & \text{at} \quad i = j. \end{cases}$$

In this case risk function (4.3) assumes the following form [137]

$$R(\delta) = C \cdot \left(1 - \sum_{i=1}^{S} p(H_i) \int_{E_i} p(x \mid H_i)\, dx\right). \tag{4.19}$$

The solution of the problem (4.19) can be written in the following way:

$$E_i = \left\{x : p(H_i)p(x \mid H_i) > p(H_j)\, p(x \mid H_j); \;\; \forall j : j \in (1,...,i-1,i+1,...,S)\right\}. \tag{4.20}$$

Let us denote

$$E_{ij} = \left\{ x : p(H_i)\, p(x \mid H_i) > p(H_j)\, p(x \mid H_j) \right\}.$$

Then

$$E_i = \bigcap_{j=1, j\neq i}^{S} E_{ij}.$$

Let us consider the case when measurement results $x_1,...,x_m$ are distributed normally, i.e. $x_i \sim N(\cdot; a_i, \sigma_i^2), i = 1,..., m$. In this case, conditional distribution density of the vector of measured values is

$$p(x \mid H_i) = \frac{1}{(2\pi)^{m/2} \prod_{\ell=1}^{m} \sigma_\ell} \exp\left\{ -\frac{1}{2} \sum_{\ell=1}^{m} \frac{\left(x_\ell - a_\ell^i\right)^2}{\sigma_\ell^2} \right\}. \tag{4.21}$$

A little manipulation yields:

$$E_{ij} = \left\{ x : \sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^j\right)}{\sigma_\ell^2} x_\ell > \lambda_{ij} \right\} \tag{4.22}$$

where

$$\lambda_{ij} = \ln \frac{p(H_j)}{p(H_i)} - \frac{1}{2} \sum_{\ell=1}^{m} \frac{\left(a_\ell^j\right)^2 - \left(a_\ell^i\right)^2}{\sigma_\ell^2}. \tag{4.23}$$

Region of hypothesis H_i acceptance

$$E_i = \left\{ x : \sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^j\right)}{\sigma_\ell^2} x_\ell \geq \lambda_{ij};\ \ \forall j : j \in (1,...,i-1,i+1,...,S) \right\}. \tag{4.24}$$

For calculation of risk function (4.19) value, it is necessary to compute the value of multidimensional integral $\int_{E_i} p(x \mid H_i) dx$. Algorithms for computation of this integral are given below.

4.3.2. Non-Step Loss Function

The solution of problem (4.3) is of the following form [133]:

$$E_j = \{x : \sum_{i=1}^{S} L(H_i, H_j)\, p(H_i)\, p(x \mid H_i) < \sum_{i=1}^{S} L(H_i, H_k)\, p(H_i)\, p(x \mid H_i); \quad \forall k : k \in (1, ..., j-1, j+1, ..., S)\}, \quad j = 1, ..., S. \tag{4.25}$$

Let us denote

$$E_{jk} = \{x : \sum_{i=1}^{S} L(H_i, H_j) p(H_i) p(x \mid H_i) < \sum_{i=1}^{S} L(H_i, H_k) p(H_i) p(x \mid H_i)\}.$$

Then

$$E_j = \bigcap_{k=1, k \neq j}^{S} E_{jk}.$$

Let us consider normally distributed measurement results, i.e. $p(x \mid H_i)$ has form (4.21). In this case, it is not difficult to obtain

$$E_{jk} = \left\{ x : \sum_{i=1}^{S-1} \lambda_{j,k}^{i} \cdot \exp\left(\sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^s\right)}{\sigma_\ell^2} x_\ell \right) < \left[L(H_s, H_k) - L(H_s, H_j) \right] \right\}, k \neq j,$$

where

$$\lambda_{j,k}^{i} = \left[L(H_i, H_j) - L(H_i, H_k) \right] \cdot \frac{p(H_i)}{p(H_S)} \cdot \exp\left\{ \frac{1}{2} \sum_{\ell=1}^{m} \frac{\left(a_\ell^s\right)^2 - \left(a_\ell^i\right)^2}{\sigma_\ell^2} \right\}.$$

Finally, for hypothesis H_i acceptance region, we have

$$E_j = \{x : \sum_{i=1}^{S-1} \lambda_{j,k}^{i} \cdot \exp\left(\sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^s\right)}{\sigma_\ell^2} x_\ell \right) < \left[L(H_S, H_k) - L(H_S, H_j) \right]; \quad \forall k : k \in \left(1, ..., j-1, j+1, ..., S\right)\}. \tag{4.26}$$

For calculation of risk function (4.3) values, it is necessary to compute the value of multidimensional integral

$$\int_{E_j} p(x \mid H_i)dx = P(x \in E_j \mid H_i)\,. \tag{4.27}$$

For its computation let us use Monte-Carlo method. Calculating time needed for this method depends on dimensionality of the integral. In hypotheses testing problem, as a rule, the number of tested hypotheses S is considerably smaller than dimensionality of the vector of measured values m, as only a small number of most likely hypotheses is left for hypotheses testing after initial processing. Therefore, to reduce the time needed for computation of integrals (4.27), we do the following.

Let us denote

$$\sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^s\right)}{\sigma_\ell^2} x_\ell = y_i, \quad i = 1,...,S-1.$$

Let us rewrite region (4.26) of acceptance of a hypothesis in the following way

$$E_j = \left\{ x : \sum_{i=1}^{S-1} \lambda_{j,k}^i \cdot \exp(y_i) < \left[I(H_S,H_k) - I(H_S,H_j) \right];\ \forall k : k \in (1,...,j-1,j+1,...,S) \right\}. \tag{4.28}$$

It is not difficult to make sure that $y = \left(y_1,...,y_{S-1}\right)$ is a normally distributed random vector with the following mathematical expectation vector and covariant matrix, correspondingly:

$$B^i = \left(b_1^i,...,b_{S-1}^i\right), \tag{4.29}$$

$$V = \begin{Vmatrix} v_{1,1}^i & v_{1,2}^i \cdots & v_{1,S-1}^i \\ v_{2,1}^i & v_{2,2}^i \cdots & v_{2,S-1}^i \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ v_{S-1,1}^i & v_{S-1,2}^i \cdots & v_{S-1,S-1}^i \end{Vmatrix}, \tag{4.30}$$

where

$$b_p^i = \sum_{\ell=1}^{m} \frac{\left(a_\ell^p - a_\ell^s\right)}{\sigma_\ell^2} \cdot a_\ell^i,$$

$$v_{p,t}^i = \sum_{\ell=1}^{m} \frac{\left(a_\ell^p - a_\ell^s\right)\left(a_\ell^t - a_\ell^s\right)}{\sigma_\ell^2}, \qquad p,t = 1,...,S-1.$$

The following equality takes place

$$\int_{E_j} p(x \mid H_i)\, dx = \int_{E_j'} p(y \mid H_i)\, dy\,, \tag{4.31}$$

where on the left side is m-dimensional integral, while on the right side -$(S-1)$-dimensional one.

The $(S-1)$-dimensionality integral in (4.31) is computed by Monte-Carlo method in the following way [133, 183]. If we simulate $(S-1)$-dimensional random vector $\xi = (\xi_1, ..., \xi_{S-1})$, where $\xi_i \sim N(\cdot;0,1)$ and $\operatorname{cov}(\xi_i, \xi_j) = 0$ at $i \neq j$, and transform it according to expression

$$\eta = B + \kappa \cdot K_1^{-1} \cdot \xi\,, \tag{4.32}$$

where B-vector of mathematical expectations, κ and K_1-matrices of eigenvectors and eigenvalues of matrix V^{-1}, correspondingly, then $\eta = (\eta_1, ..., \eta_{S-1})$ will be a normally distributed random vector with mathematical expectation B and covariant matrix V.

Assume that n values of random vector η were computed according to relation (4.32), and ν of them belong to region (4.30). Then

$$\hat{p} = \frac{\nu}{n}$$

is an estimate of integral (4.31) value, computed by Monte-Carlo method.

The size of played random vectors, that provides δ-accuracy of integral computation with likelihood $(1-\alpha)$, is defined by the following relation

$$n = \left\lfloor \frac{1}{4\alpha\delta^2} \right\rfloor,$$

where $\left\lfloor \frac{1}{4\alpha\delta^2} \right\rfloor$ is the minimum integer number $\geq \frac{1}{4\alpha\delta^2}$.

To minimize the number of generated random vectors that are necessary for computation values of integral (4.31) with specified accuracy, we do the following. We deliberately specify a rough accuracy of integral (4.31) computation $\delta_1 > \delta$, and for sample size

$$n_1 = \left\lfloor \frac{1}{4\alpha_1\delta_1^2} \right\rfloor,$$

where $\alpha_1 \le \alpha$, compute estimate $\hat{p}_{n_1}$. The final sample size is calculated according to relation

$$n = \max_{p \in [\bar{p}_{n_1} - \delta_1; \bar{p}_{n_1} + \delta_1]} \left[\frac{p(1-p)}{\alpha \delta^2} \right]. \tag{4.33}$$

This enables to reduce substantially the time needed for the probability integral computation, when it considerably differs from 0.5.

For calculation of eigenvalues and eigenvectors of matrix V^{-1}, matrix V is required to be positively definite. A correlation matrix is always positively definite. Therefore, it is necessary to go over from covariant matrix V to the correlation one by normalizing the elements of matrix V. Let us show the changes entailed by going over to the correlation matrix, when calculating integrals (4.31) by Monte-Carlo method.

Let us introduce the following denotation:

$$z_p = \frac{y_p}{\sqrt{D(y_p)}} = \frac{y_p}{\sqrt{v^i_{p,p}}}, \tag{4.34}$$

i.e.

$$\begin{aligned} E(z_p \mid H_i) &= \frac{b_p}{\sqrt{v^i_{p,p}}} \\ E(z_p z_k \mid H_i) &= \frac{E(y_p y_k \mid H_i)}{\sqrt{V(y_p \mid H_i) \cdot V(y_k \mid H_i)}} = \frac{v^i_{p,k}}{\sqrt{v^i_{p,p}} \cdot \sqrt{v^i_{k,k}}}. \end{aligned} \tag{4.35}$$

In these denotations, (4.31) may be rewritten in the following way .

$$\begin{aligned} \int_{E_j} p(x \mid H_i) dx &= \left(\prod_{p=1, p \ne i}^{S} \sqrt{v^i_{p,p}} \right) \cdot \\ \int_{E_j^*} (2\pi)^{-(S-1)/2} \cdot |V|^{-1/2} &\exp\left\{ -\frac{1}{2} (D \cdot z - B_i)^T \cdot V^{-1} \cdot (D \cdot z - B_i) \right\} dz, \end{aligned} \tag{4.36}$$

where

$$D = \begin{pmatrix} \sqrt{v^i_{1,1}}\,0.....0 \\ ..... \\ 0.....0\ \sqrt{v^i_{i-1,i-1}}\ 0.....0 \\ 0.....0\ \sqrt{v^i_{i+1,i+1}}\ 0.....0 \\ ..... \\ 0.....0\ \sqrt{v^i_{S,S}} \end{pmatrix},$$

$$E^i_j = \left\{ z : \sum_{i=1}^{S-1} v^i_{j,k} \exp\left(\sqrt{v^i_{j,j}} \cdot z_j\right) < \left[L(H_S, H_k) - L(H_S, H_j) \right]; \forall k : k \in (1,...,j-1,j+1,...,S) \right\}. \quad (4.37)$$

Let us rewrite (4.36) in the following form:

$$\int_{E_j} p(x \mid H_i)\, dx = \left(\prod_{p=1, p \neq i}^{S} \sqrt{v^i_{p,p}} \right) \cdot \int_{E^i_j} (2\pi)^{-(S-1)/2} \cdot |V|^{-1/2} \cdot |D| \cdot \exp\left\{ -\frac{1}{2} \left(z - D^{-1} B_i\right)^T \cdot D^T \cdot V^{-1} \cdot D \cdot (z - D^{-1} B_i) \right\} dz. \quad (4.38)$$

Let us denote $D^{-1} B_i = B'_i$, $D^T V^{-1} D = W^{-1}$. Then (4.38) may be rewritten as

$$\int_{E_j} p(x \mid H_i) dx = \int_{E^i_j} (2\pi)^{-(S-1)/2} \ |W|^{-1/2} \exp\left\{ -\frac{1}{2} \left(z - B'_i\right)^T \ W^{-1} \ \left(z - B'_i\right) \right\} dz. \quad (4.39)$$

Thus, for computation of integrals (4.31), it is necessary to simulate normally distributed $(S-1)$-dimensional random vector z with mathematical expectation B'_i and correlation matrix W, and if this vector satisfies (4.37), to consider that we are in the domain of integration and to increase the value of ν by one.

Let us give another more reliable from computational point of view, way of computation of integrals (4.27). By "reliable" we mean that, in this case, no inversion of covariant matrices and finding of their eigenvalues and eigenvectors is required.

Let us rewrite hypotheses testing regions (4.25) in the following way

$$E_j = \{ x : \sum_{p=1}^{S} [L(H_p, H_j) - L(H_p, H_k)]\, p(H_p)\, p(x \mid H_p) < 0; \quad \forall k : k \in (1,..., j-1, j+1,..., S) \}. \quad (4.40)$$

For normal probability distribution density (4.21), expression (4.40) assumes the following form

$$E_j = \{x : C \cdot \sum_{p=1}^{S} [L(H_p, H_j) - L(H_p, H_k)] \cdot p(H_p) \cdot \exp\left\{ -\frac{1}{2} \sum_{\ell=1}^{m} \frac{\left(x_\ell - a_\ell^p\right)^2}{\sigma_\ell^2} \right\} < 0; \quad \forall k : k \in (1,...,j-1,j+1,...,S)\}, \tag{4.41}$$

where $C = 1 / \left[\left(2\pi\right)^{m/2} \prod_{\ell=1}^{m} \sigma_\ell \right]$.

Random quantity

$$y_p = \sum_{\ell=1}^{m} \frac{\left(x_\ell - a_\ell^p\right)^2}{\sigma_\ell^2}, \quad p = 1,...,S, \tag{4.42}$$

is distributed according to χ^2-probability distribution law with variance m and non-centrality parameter

$$\gamma_p = \sum_{\ell=1}^{m} \frac{\left(a_\ell^i - a_\ell^p\right)^2}{\sigma_\ell^2}, \quad p = 1,...,S, \tag{4.43}$$

at hypotheses H_i truth. Therefore, for computation of probability integral (4.27), we n times generate S random quantities (4.42) with non-centrality parameters (4.43) and assign to ν the value which is equal to the number of times these vectors will satisfy condition (4.41). Probability integral (4.27) value is defined according to formula (4.33).

It should be also noted, that, when using the above algorithms for many hypotheses testing, mathematical expectations a_i, $i = 1,...,N$, of measured parameters and the parameters themselves may take arbitrary values, depending on special features of practical problems solved. To avoid undesired aferrunnings in calculation process, caused by computer registers overflow or appearance of computer zeros, it is reasonable to normalize initial data.

Let c_j and d_j, $j = 1,...,m$, denote, correspondingly, the minimum and the maximum values of the j th coordinate of all the points of mathematical expectations of measurement results, i.e.

$$c_j = \min_{\{i\}}\left(a_{ij}\right), \quad d_j = \min_{\{i\}}\left(a_{ij}\right), \quad j = 1,...,m.$$

Instead of points a_i, $i = 1,...,S$, let us consider points b_i, $i = 1,...,S$, with coordinates $b_i(b_{i_1}, b_{i_2},..., b_{i_m})$, where

$$b_{ij} = \left(a_{ij} - c_j\right) / \left(d_j - c_j\right), \quad j = 1,...,m; \quad i = 1,...,S.$$

Measurement results and their variances will be accordingly recalculated

$$x_j^{'} = \left(x_j - c_j\right) / \left(d_j - c_j\right), \quad \sigma_j^{'2} = \sigma_j^2 / \left(d_j - c_j\right)^2, \quad j = 1,...,m.$$

4.4. ALGORITHMS OF SOLVING CONDITIONAL BAYESIAN PROBLEM OF MANY SIMPLE HYPOTHESES TESTING

One of generalizations of the classical statement of Bayesian problem of many hypotheses testing given in paragraph 4.1 consists in the solution of conditional optimization problem instead of unconditional one, which enables to make guaranteed decisions with respect to errors of true decision rejections. Below, the general solution of conditional Bayesian problem at restrictions on the averaged probability of omitted true parameters is brought up to the computational algorithms for the most common in practice, normal distribution of probabilities of measurement results.

As an example of elaboration of algorithms of the decision of conditional Bayesian task of test of many hypotheses let us consider the task (4.9), (4.14). The solution of this problem is (4.15). Let us consider the case when measurement results $x_1,...,x_m$ are distributed normally, i.e. looks like (4.21). Subject to (4.21), hypothesis H_i acceptance region (4.15) may be rewritten in the following way

$$E_i = \left\{ x : \sum_{j=1, j\neq i}^{S} \lambda_{ij} \cdot \exp\left(\sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} x_\ell \right) < \lambda \right\}, \tag{4.48}$$

where

$$\lambda_{ij} = \frac{p(H_j)}{p(H_i)} \cdot \exp\left\{ \frac{1}{2} \sum_{\ell=1}^{m} \frac{\left(a_\ell^i\right)^2 - \left(a_\ell^j\right)^2}{\sigma_\ell^2} \right\}.$$

To find values of unknown coefficient λ so as to hold equality in (4.14), computation of the following integrals

$$\int_{E_i} p(x \mid H_i)\, dx = P(x \in E_i \mid H_i) = P\left(\sum_{j=1, j\neq i}^{S} \lambda_{ij} \cdot \exp\left\{ \sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} x_\ell \right\} < \lambda \mid H_i \right) \tag{4.49}$$

is required with high accuracy, since otherwise it will be impossible to hold equality in condition (4.14) with required accuracy, i.e. to ensure the required quality of decision rule (4.15).

Let us denote

$$\varsigma_i = \sum_{j=1, j\neq i}^{S} \lambda_{ij} \cdot \exp\left\{ \sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} x_\ell \right\},$$

and by $p_i(z \mid H_i)$ -its conditional probability distribution density

$$\int_{E_i} p(x \mid H_i)dx = \int_0^{\lambda} p_i(z \mid H_i)dz.$$

The range of integration is taken from 0 to $+\infty$, since $0 < p(H_i) \leq 1$, $0 < \lambda \leq 1$, $\lambda_{ij} > 0$.

Random quantity ς_i is the weighted sum of log-normally distributed random quantities. Therefore, it is impossible, to find analytical expression of its density [133, 183]. Let us consider the possibility of this density approximation by series.

Random vector $y = (y_1, ..., y_{S-1})$, components of which

$$y_j = \sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} x_\ell, \quad j = 1, ..., S; \quad j \neq i,$$

are dependent, normally distributed random quantities, at hypothesis H_i truth, has $(S-1)$-dimensional conditional normal probability distribution density with mathematical expectation vector $B_i^T = (b_1^i, ..., b_{S-1}^i)$ and dispersion matrix

$$\sum = \begin{Vmatrix} k_{1,1}^i & k_{1,2}^i \ldots\ldots\ldots\ldots k_{1,S-1}^i \\ k_{2,1}^i & k_{2,2}^i \ldots\ldots\ldots\ldots k_{2,S-1}^i \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ k_{S-1,1}^i & k_{S-1,2}^i \qquad\qquad k_{S-1,S-1}^i \end{Vmatrix},$$

where

$$b_p^i = \sum_{\ell=1}^{m} \frac{a_\ell^p - a_\ell^i}{\sigma_\ell^2} \cdot a_\ell^i,$$

$$k_{p,t}^i = \sum_{\ell=1}^{m} \frac{\left(a_\ell^p - a_\ell^i\right)\left(a_\ell^t - a_\ell^i\right)}{\sigma_\ell^2}, \quad p,t = 1,...,S; \quad p \neq i; \quad t \neq i.$$

Let us calculate the r th initial moment of random quantity ς_i, on condition that hypothesis H_i is true

$$\mu_r^i = E\left[\varsigma_i^r \mid H_i\right] = E\left[\left(\sum_{j=1, j\neq i}^{S} \lambda_{ij} \cdot \exp\left(y_j\right)\right)^r \mid H_i\right] =$$

$$= \sum_{j_1=1, j_1\neq i}^{S} ... \sum_{j_r=1, j_r\neq i}^{S} \lambda_{i,j_1} ... \lambda_{i,j_r} \cdot E\left[\exp\left(y_{j_1} + ... + y_{j_r}\right) \mid H_i\right].$$

Let us denote: $u_{j_1,...,j_r} = y_{j_1} + ... + y_{j_r}$. Mathematical expectation of log-normally distributed random quantity $\exp\left(u_{j_1,...,j_r}\right)$, at truth of H_i is [102, 133, 142, 183]

$$E\left[\exp\left(u_{j_1,...,j_r}\right) \mid H_i\right] = \exp\left\{\frac{1}{2} \cdot V\left(u_{j_1,...,j_r} \mid H_i\right) + E\left(u_{j_1,...,j_r} \mid H_i\right)\right\}.$$

It is not difficult to find

$$E\left(u_{j_1,...,j_r} \mid H_i\right) = \sum_{\ell=1}^{r} b_{j_\ell}^i$$

$$V\left(u_{j_1,...,j_r} \mid H_i\right) = \sum_{p,t=j_1,...,j_r} k_{p,t}^i.$$

,

Finally

$$\mu_r^i = \sum_{j_1=1, j_1\neq i}^{s} ... \sum_{j_r=1, j_r\neq i}^{s} \lambda_{i,j_1} ... \lambda_{i,j_r} \cdot \exp\left\{\frac{1}{2} \cdot V\left(u_{j_1,...,j_r} \mid H_i\right) + E\left(u_{j_1,...,j_r} \mid H_i\right)\right\}.$$

Since ς_j is a positively definite random quantity, we shall use Laguerre polynomials for its density approximation [130, 141, 144]. Probability distribution density $p_i(z \mid H_i)$ may be formally expanded into a series [130, 141]

$$p_i(z \mid H_i) = \sum_{n=0}^{\infty} C_n^i \cdot p_n(z) \cdot f(z) \quad , \tag{4.50}$$

where:

$$p_n(z) = \frac{L_n^{(\gamma)}(z)}{\sqrt{\frac{(n+\gamma-1)!}{(\gamma-1)!n!}}}$$

is a sequence of orthogonal polynomials connected with the distribution defined by Pearson density function of the III-rd kind [130];

$$f(z,\gamma) = \begin{cases} \frac{1}{\Gamma(\gamma)} z^{\gamma-1} e^{-z}, & \text{when} \quad z > 0, \\ 0, & \text{when } z \le 0; \end{cases}$$

$\Gamma(\gamma) = \int_0^{\infty} z^{\gamma-1} e^{-z} dz$ - gamma function, $\gamma > 0$ [142, 184]; $L_n^{(\gamma)}(z)$ -Laguerre polynomials that are defined by the following relation [109, 130, 185]:

$$\left(\frac{d}{dz}\right)^n \left(z^{n+\gamma-1} e^{-z}\right) = (-1)^n \, n! \, L_n^{(\gamma)}(z) \cdot z^{\gamma-1} \cdot e^{-z} . \tag{4.51}$$

The orthogonality condition for coefficients C_n^i gives [130, 141]:

$$C_n^i = \int_0^{\infty} p_n(z) \, p_i(z \mid H_i) \, dz . \tag{4.52}$$

Using relation (4.51) for Laguerre polynomials, we'll obtain:

$$L_0^{(\gamma)}(z) = 1$$
$$L_1^{(\gamma)}(z) = z - \gamma$$
$$L_2^{(\gamma)}(z) = \frac{1}{2}\left[z^2 - 2(\gamma+1)z + (\gamma+1)\gamma\right]$$
$$L_3^{(\gamma)}(z) = \frac{1}{6}\left[z^3 - 3(\gamma+2)z^2 + 3(\gamma+2)(\gamma+1)z - (\gamma+2)(\gamma+1)\gamma\right]$$

$$L_4^{(\gamma)}(z)=\frac{1}{24}[z^4-4(\gamma+3)z^3+6(\gamma+3)(\gamma+2)z^2-4(\gamma+3)(\gamma+2)(\gamma+1)z+$$
$$+(\gamma+3)(\gamma+2)(\gamma+1)\gamma] \tag{4.53}$$
$$L_5^{(\gamma)}(z)=\frac{1}{120}[z^5-5(\gamma+4)z^4+10(\gamma+4)(\gamma+3)z^3-10(\gamma+4)(\gamma+3)(\gamma+2)z^2+$$
$$+5(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)z-(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)\gamma].$$

According to relation (4.52) for coefficients C_n^i, we'll obtain:

$$C_0^i=1$$
$$C_1^i=\frac{1}{\sqrt{\gamma}}(\mu_1^i-\gamma)$$
$$C_2^i=\frac{1}{\sqrt{2\gamma(\gamma+1)}}(\mu_2^i-2(\gamma+1)\mu_1^i+(\gamma+1)\gamma)$$
$$C_3^i=\frac{1}{\sqrt{6\gamma(\gamma+1)(\gamma+2)}}(\mu_3^i-3(\gamma+2)\mu_2^i+3(\gamma+2)(\gamma+1)\mu_1^i-(\gamma+2)(\gamma+1)\gamma) \tag{4.54}$$
$$C_4^i=\frac{1}{\sqrt{24\gamma(\gamma+1)(\gamma+2)(\gamma+3)}}(\mu_4^i-4(\gamma+3)\mu_3^i+6(\gamma+3)(\gamma+2)\mu_2^i-4(\gamma+3)(\gamma+2)\cdot$$
$$\cdot(\gamma+1)\mu_1^i+(\gamma+3)(\gamma+2)(\gamma+1)\gamma)$$
$$C_5^i=\frac{1}{\sqrt{120\gamma(\gamma+1)(\gamma+2)(\gamma+3)(\gamma+4)}}(\mu_5^i-5(\gamma+4)\mu_4^i+10(\gamma+4)(\gamma+3)\mu_3^i-$$
$$-10(\gamma+4)(\gamma+3)(\gamma+2)\mu_2^i+5(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)\mu_1^i-(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)\gamma).$$

Subject to (4.53), (4.54), expansion (4.50) assumes the following form:

$$p_i(z\mid H_i)=f(z,\gamma)+\frac{1}{\gamma}(\mu_1^i-\gamma)(z-\gamma)f(z,\gamma)+$$
$$+\frac{1}{2\gamma(\gamma+1)}(\mu_2^i-2(\gamma+1)\mu_1^i+(\gamma+1)\gamma)(z^2-2(\gamma+1)z+(\gamma+1)\gamma)f(z,\gamma)+$$
$$+\frac{1}{6\gamma(\gamma+1)(\gamma+2)}(\mu_3^i-3(\gamma+2)\mu_2^i+3(\gamma+2)(\gamma+1)\mu_1^i-(\gamma+2)(\gamma+1)\gamma)\cdot$$
$$\cdot(z^3-3(\gamma+2)z^2+3(\gamma+2)(\gamma+1)z-(\gamma+2)(\gamma+1)\gamma)f(z,\gamma)+$$
$$+\frac{1}{24\gamma(\gamma+1)(\gamma+2)(\gamma+3)}(\mu_4^i-4(\gamma+3)\mu_3^i+6(\gamma+3)(\gamma+2)\mu_2^i-4(\gamma+3)(\gamma+2)\cdot$$
$$\cdot(\gamma+1)\mu_1^i+(\gamma+3)(\gamma+2)(\gamma+1)\gamma)\cdot(z^4-4(\gamma+3)z^3+6(\gamma+3)(\gamma+2)z^2-4(\gamma+3)\cdot$$

$$\cdot(\gamma+2)(\gamma+1)z+(\gamma+3)(\gamma+2)(\gamma+1)\gamma)f(z,\gamma)+\frac{1}{120\gamma(\gamma+1)(\gamma+2)(\gamma+3)(\gamma+4)}\cdot$$
$$\cdot(\mu_5^j-5(\gamma+4)\mu_4^j+10(\gamma+4)(\gamma+3)\mu_3^j-10(\gamma+4)(\gamma+3)(\gamma+2)\mu_2^j+5(\gamma+4)(\gamma+3)\cdot$$
$$\cdot(\gamma+2)(\gamma+1)\mu_1^j-(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)\gamma)\cdot(z^5-5(\gamma+4)z^4+10(\gamma+4)(\gamma+3)z^3-$$
$$-10(\gamma+4)(\gamma+3)\cdot(\gamma+2)z^2+5(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)z-(\gamma+4)(\gamma+3)(\gamma+2)\cdot$$
$$\cdot(\gamma+1)\gamma)f(z,\gamma)+... \qquad (4.55)$$

Let $G_i(z\,|\,H_i)$ denote conditional function of random quantity ς_i distribution, and let $F(z,\gamma)$ denote the probability distribution function corresponding to density $f(z,\gamma)$, i.e.

$$F(z,\gamma)=\frac{1}{\Gamma(\gamma)}\int_0^z x^{\gamma-1}e^{-x}dx.$$

Then, taking into account (4.51) and (4.55), we'll obtain

$$G_i(z\,|\,H_i)=F(z,\gamma)-\frac{1}{\gamma}(\mu_1^j-\gamma)zf(z,\gamma)+\frac{1}{2\gamma(\gamma+1)}(\mu_2^j-2(\gamma+1)\mu_1^j+$$
$$+(\gamma+1)\gamma)(-z^2+(\gamma+1)z)f(z,\gamma)-\frac{1}{6\gamma(\gamma+1)(\gamma+2)}(\mu_3^j-3(\gamma+2)\mu_2^j+$$
$$+3(\gamma+2)(\gamma+1)\mu_1^j-(\gamma+2)(\gamma+1)\gamma)\cdot(z^3-2(\gamma+2)z^2+(\gamma+2)(\gamma+1)z)f(z,\gamma)+$$
$$+\frac{1}{24\gamma(\gamma+1)(\gamma+2)(\gamma+3)}(\mu_4^j-4(\gamma+3)\mu_3^j+6(\gamma+3)(\gamma+2)\mu_2^j-4(\gamma+3)(\gamma+2)$$
$$\cdot(\gamma+1)\mu_1^j+(\gamma+3)(\gamma+2)(\gamma+1)\gamma)\cdot(-z^4+3(\gamma+3)z^3-3(\gamma+3)(\gamma+2)z^2+(\gamma+3)\cdot$$
$$\cdot(\gamma+2)(\gamma+1)z)f(z,\gamma)-\frac{1}{120\gamma(\gamma+1)(\gamma+2)(\gamma+3)(\gamma+4)}\cdot(\mu_5^j-5(\gamma+4)\mu_4^j+$$
$$+10(\gamma+4)(\gamma+3)\mu_3^j-10(\gamma+4)(\gamma+3)(\gamma+2)\mu_2^j+5(\gamma+4)(\gamma+3)\cdot(\gamma+2)(\gamma+1)\mu_1^j- \qquad (4.56)$$
$$-(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)\gamma)\cdot(z^5-4(\gamma+4)z^4+6(\gamma+4)(\gamma+3)z^3-$$
$$-4(\gamma+4)(\gamma+3)\cdot(\gamma+2)z^2+(\gamma+4)(\gamma+3)(\gamma+2)(\gamma+1)z)f(z,\gamma)+...$$

Concerning of convergence of expansion (4.56), there is a theorem that states [184]: if $G_i(z\,|\,H_i)$ is a continuous function on semi-axis $z\ge 0$ and $G_i(z\,|\,H_i)=0(z^m)$ at $z\to+\infty$, where m is an arbitrary fixed positive number, and $\left|G_i'(z\,|\,H_i)\right|=\left|p_i(z\,|\,H_i)\right|<A$, where A is constant, then, at $\gamma<0$, expansion (4.56) converges to $G_i(z\,|\,H_i)$ on the interval $0\le z\le\omega$. Since $G_i(z\,|\,H_i)$ is a probability distribution function, the theorem conditions are satisfied. Therefore, series (4.56) converges.

To find unknown λ value in solution (4.48), the algorithm of dividing in half is used. The essence of the problem consists in the following. Initial approximations λ_B and λ_H are taken so as to hold $\hat{F}(E(\lambda_B)) < 1-\alpha$ and $\hat{F}(E(\lambda_H)) > 1-\alpha$, were the following designation is introduced

$$F(E(\lambda)) = \sum_{i=1}^{S} p(H_i) \int_{E_i} p(x \mid H_i) dx$$

and the sign over F shows that it is an estimation of the corresponding true value.

The desired value of λ is calculated in the following way

$$\lambda = \left(\lambda_B + \lambda_H\right) / 2 . \tag{4.57}$$

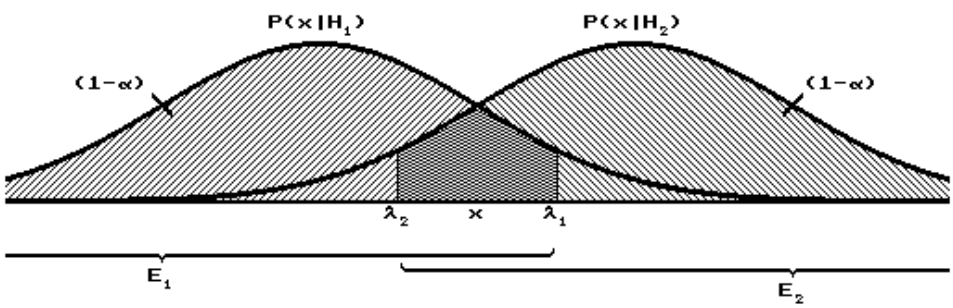
The following condition is tested

$$\frac{\left|\hat{F}(E(\lambda)) - (1-\alpha)\right|}{\hat{F}(E(\lambda))} \le \delta , \tag{4.58}$$

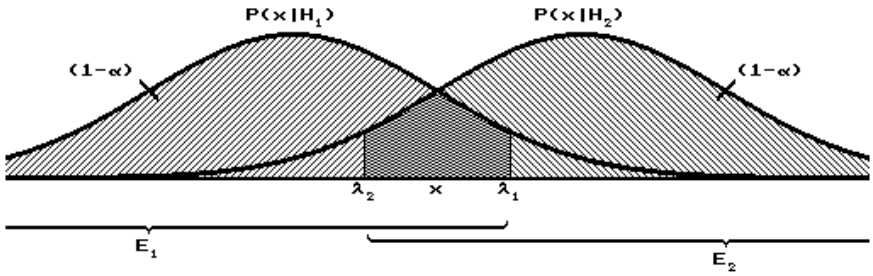
where δ -the accuracy of Eq. (4.14) solution.

If (4.58) holds, then the value of λ is considered found with the specified accuracy, a decision is made on conditions (4.48), and the corresponding value of risk function is calculated according to formula (4.9) in which the integral values are computed by means of expansion (4.56).

If (4.58) doesn't hold, condition $\hat{F}(E(\lambda)) < 1-\alpha$ is tested. If it is satisfied, then assignment $\lambda_B := \lambda$, otherwise $\lambda_H := \lambda$, is carried out. A new approximation is calculated by formula (4.57) and so on until condition (4.58) is fulfilled.



(a)



(b)

Figure 4.1. Diagrammatic representation of decision-making ambiguity.

The integral values entering into $F(E(\lambda))$ are computed by expansion (4.56).

When solving practical problems, the following non-trivial situations are possible. When hypotheses are near to each other, the situation shown in Figure 4.1(a) may take place. This means that it is impossible to make decision in this situation with the specified power of $(1-\alpha)$. And when the measurement result falls into the interval between λ_2 and λ_1, it is impossible to make one decision. In that case, it is necessary to decrease power of criterion $(1-\alpha)$ until hypothesis acceptance regions are separated. The criterion power will be equal to the value to which correspond non-intersectional regions.

On the other hand, when hypotheses are separated from each other, the situation shown in Figure 4.1(b) may take place. This means that, when the measurement result falls between λ_1 and λ_2, it is impossible to make a decision. In this case, it is necessary to increase power of criterion $(1-\alpha)$ until the measured value is found in one of the regions of hypothesis acceptance. The criterion power will be equal to the corresponding value.

4.5. SOLUTION OF UNCONDITIONAL BAYESIAN PROBLEM AT NUMBER OF HYPOTHESES EQUAL TO TWO

The finding of optimum regions of hypotheses testing in unconditional and conditional Bayesian problems of testing many hypotheses and computation of suitable values of risk function is connected with complex problem of repeated computation of multidimensional probability integrals on the regions of complex configuration in iterative process of finding unknown Lagrange coefficients. The problem is considerably simplified if number of hypotheses $S=2$. In this case, the finding of optimum regions of acceptance of hypotheses and computation of risk function is possible analytically. Therefore for those cases, when as a result of working of an algorithm of formation of hypotheses, the number of formed hypotheses is equal to two, below is offered simple algorithm.

In this case, risk function (4.3) is of the following form:

$$R(S=2)=L(H_1,H_2).P(H_1)\int_{E_2}P(x|H_1)dx+L(H_2,H_1).P(H_2)\int_{E_1}P(x|H_2)dx\Rightarrow\min_{\{E_1,E_2\}}. \tag{4.58}$$

It is obvious that condition $L(H_1, H_2) = L(H_2, H_1) = C$ hold, i.e. at $S = 2$, only a step loss function may take place. Let us rewrite (4.58 in the following way

$$R(S=2) = C.\left[P(H_1) \int_{E_2} P(x \mid H_1)dx + P(H_2) \int_{E_1} P(x \mid H_2)dx \right] \Rightarrow \min_{\{E_1, E_2\}}. \quad (4.59)$$

The minimum in (4.59) is reached in the following hypotheses-acceptance regions

$$E_1 = \{x : P(H_1) \cdot P(x \mid H_1) > P(H_2) \cdot P(x \mid H_2)\},$$
$$E_2 = \{x : P(H_2) \cdot P(x \mid H_2) > P(H_1) \cdot P(x \mid H_1)\}.$$

Subject to (4.21), for hypotheses-acceptance regions, we finally obtain

$$E_1 = \left\{ x : \sum_{\ell=1}^{m} \frac{a_\ell^2 - a_\ell^1}{\sigma_\ell^2} \cdot x_\ell < \lambda_1 \right\}, \quad E_2 = \left\{ x : \sum_{\ell=1}^{m} \frac{a_\ell^1 - a_\ell^2}{\sigma_\ell^2} \cdot x_\ell < \lambda_2 \right\},$$

where

$$\lambda_1 = \ln \frac{p(H_1)}{p(H_2)} - \frac{1}{2} \cdot \sum_{\ell=1}^{m} \frac{(a_\ell^1)^2 - (a_\ell^2)^2}{\sigma_\ell^2},$$
$$\lambda_2 = \ln \frac{p(H_2)}{p(H_1)} - \frac{1}{2} \cdot \sum_{\ell=1}^{m} \frac{(a_\ell^2)^2 - (a_\ell^1)^2}{\sigma_\ell^2}.$$

The risk function value is calculated analytically

$$R(\delta=2) = C \cdot \left[p(H_1) \cdot \Phi \left(\frac{\ln \frac{p(H_2)}{p(H_1)} - \frac{1}{2} \cdot \sum_{\ell=1}^{m} \frac{(a_\ell^2)^2 - (a_\ell^1)^2}{\sigma_\ell^2} - \sum_{\ell=1}^{m} \frac{(a_\ell^1 - a_\ell^2)}{\sigma_\ell^2} \cdot a_\ell^1}{\sqrt{\sum_{\ell=1}^{m} \frac{(a_\ell^2 - a_\ell^1)^2}{\sigma_\ell^2}}} \right) + \right.$$
$$\left. + p(H_2) \cdot \Phi \left(\frac{\ln \frac{p(H_1)}{p(H_2)} - \frac{1}{2} \cdot \sum_{\ell=1}^{m} \frac{(a_\ell^1)^2 - (a_\ell^2)^2}{\sigma_\ell^2} - \sum_{\ell=1}^{m} \frac{(a_\ell^2 - a_\ell^1)}{\sigma_\ell^2} \cdot a_\ell^2}{\sqrt{\sum_{\ell=1}^{m} \frac{(a_\ell^2 - a_\ell^1)^2}{\sigma_\ell^2}}} \right) \right],$$

where Φ – is standard normal function of probabilities distribution.

4.6. Solution of Conditional Bayesian Problem at Number of Hypotheses Equal to Two

In this case conditional Bayesian problem becomes

$$r_\delta(s=2) = p(H_1)\int\limits_{E_2} p(x \mid H_1)dx + p(H_2)\int\limits_{E_1} p(x \mid H_2)dx \Rightarrow \min\limits_{\underline{\{E_1,E_2\}}}, \tag{4.60}$$

under condition of

$$\int\limits_{E_1} p(x \mid H_1)dx \geq (1-\alpha), \quad \int\limits_{E_2} p(x \mid H_2)dx \geq (1-\alpha). \tag{4.61}$$

The optimization problem (4.60), (4.61) is divided into two independent problems

$$\int\limits_{E_i} p(x \mid H_j)dx \Rightarrow \min\limits_{\{E_i\}}, \tag{4.62}$$

under condition of

$$\int\limits_{E_i} p(x \mid H_i)dx \geq (1-\alpha), \quad i,j = 1,2; \quad i \neq j. \tag{4.63}$$

The optimum solutions of these problems are given by the rule of Neumann-Pearson

$$E_1 = \{x : \frac{p(x \mid H_2)}{p(x \mid H_1)} < \lambda_1\}, \quad E_2 = \{x : \frac{p(x \mid H_1)}{p(x \mid H_2)} < \lambda_2\},$$

where λ_1, λ_2 are determined so that in conditions (4.63) the equality took place.

For a normal probability distribution law the optimum regions of acceptance of hypotheses become

$$E_1 = \left\{x : \sum_{\ell=1}^{m} \frac{a_\ell^2 - a_\ell^1}{\sigma_\ell^2} \cdot x_\ell \leq \lambda_1\right\}, \quad E_2 = \left\{x : \sum_{\ell=1}^{m} \frac{a_\ell^1 - a_\ell^2}{\sigma_\ell^2} \cdot x_\ell \leq \lambda_2\right\},$$

where

$$\lambda_1 = \Phi^{-1}(1-\alpha) \cdot \sqrt{\sum_{\ell=1}^{m} \frac{(a_\ell^2 - a_\ell^1)^2}{\sigma_\ell^2}} + \sum_{\ell=1}^{m} \frac{(a_\ell^2 - a_\ell^1)}{\sigma_\ell^2} \cdot a_\ell^1,$$

$$\lambda_2 = \Phi^{-1}(1-\alpha) \cdot \sqrt{\sum_{\ell=1}^{m} \frac{(a_\ell^1 - a_\ell^2)^2}{\sigma_\ell^2}} + \sum_{\ell=1}^{m} \frac{(a_\ell^1 - a_\ell^2)}{\sigma_\ell^2} \cdot a_\ell^2,$$

$\Phi^{-1}(\cdot)$ is inverse of the standard normal probability distribution function.

The value of the average risk is calculated under the formula

$$r_\delta(S=2)=\Phi(\Phi^{-1}(1-\alpha)-\sqrt{G}),$$

where

$$G=\sqrt{\sum_{\ell=1}^{m}\frac{(a_\ell^1-a_\ell^2)^2}{\sigma_\ell^2}}.$$

4.7. QUASI-OPTIMAL METHOD OF MANY-HYPOTHESES TESTING

Finding of regions of acceptance of hypotheses in conditional Bayesian problem of hypotheses testing and calculation of the corresponding values of a risk function is the difficult task requiring of iterative calculation of multidimensional normal integrals on the integrating areas of the complex configuration [133, 183]. At the solution of practical problems often it is necessary to have the simple, not optimum decision rules no requiring of large computer and computing resources for their calculation.

Such quasi-optimal algorithms for solution of problems (4.8), (4.10), for intersectional and for non-intersectional hypotheses are given in [133]. Let us consider solution of problem (4.9), (4.14).

For solution of problem (4.9), (4.14), let us consider $S-1$ particular problems of the following type: we must test the null hypothesis that supposes the truth of H_i against that supposes the truth of H_j, $j=1,...,S$, $j\neq i$. Let E_{ij} denote the region of hypothesis H_i acceptance when testing two hypotheses H_i and H_j, then the problem will have the following analytical form:

$$\int_{E_{ij}} p(x\mid H_j)\,dx \Rightarrow \min_{E_{ij}}, \tag{4.59}$$

on condition that

$$\int_{E_{ij}} p(x\mid H_i)dx \geq \beta, \quad j=1,...,S, \quad j\neq i, \tag{4.60}$$

where β is chosen so as to hold equality in (4.14), i.e. the probability of hypothesis H_i acceptance at its truth will be not less than the specified level.

The solution of problem (4.59), (4.60) is given by Neumann-Pearson criterion, according to which the critical region has the following form:

$$E_{ij} = \left\{ x : \frac{p(x \mid H_j)}{p(x \mid H_i)} \le \lambda_{ij} \right\},$$

where λ_{ij} is defined so as to hold equality in (4.60).

Hypotheses H_i acceptance region is of the following form

$$E_i = \bigcap_{j=1, j\neq i}^{S} E_{ij},$$

i.e.

$$E_i = \left\{ x : \frac{p(x \mid H_j)}{p(x \mid H_i)} \le \lambda_{ij}, \forall j : j \in (1,...,i-1,i+1,...,S) \right\}.$$

As mentioned above, the condition of determination of threshold λ_{ij} is so as in (4.60) the equality took place. Let us define β so as to satisfy the condition (4.14). Really

$$\sum_{i=1}^{S} p(H_i) \int_{E_i} p(x \mid H_i) dx = 1 - \sum_{i=1}^{S} p(H_i) \cdot p(x \in \overline{E_i} \mid H_i) >$$

$$> 1 - \sum_{i=1}^{S} p(H_i) \sum_{i=1, j\neq i}^{S} p(x \in \overline{E}_{ij} \mid H_i) = 1 - \sum_{i=1}^{S} p(H_i) \cdot \sum_{j=1, j\neq i}^{S} [1 -$$

$$- P(x \in \mathrm{E}_{ij} \mid H_i)] = 1 - \sum_{i=1}^{S} p(H_i) \cdot [(S-1) + \sum_{j=1, j\neq i}^{S} P(x \in \mathrm{E}_{ij} \mid H_i)] =$$

$$= 1 - (S-1)(1-\beta).$$

It is obvious that, if we take

$$\beta = 1 - \frac{\alpha}{S-1},$$

condition (4.14) will always hold.

It is not difficult to obtain for probability distribution density (4.21)

$$\tilde{E}_i = \left\{ x : \sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} \cdot x_\ell \le \tilde{\lambda}_{ij}; \forall j : j \in (1,...,i-1,i+1,...,S) \right\}, \quad i = 1,...,S,$$

where

$$\tilde{\lambda}_{ij} = \Phi^{-1}(\beta) \sqrt{\sum_{\ell=1}^{m} \frac{\left(a_\ell^j - a_\ell^i\right)^2}{\sigma_\ell^2}} + \sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} \cdot a_\ell^i,$$

where $\Phi^{-1}(\cdot)$ - the inverse standard normal function of probability distribution.

Taking into consideration the statement of quasi-optimal problem, the corresponding expression for risk function will be of the following form:

$$r(\delta) = \sum_{j=1}^{S} p(H_j) \cdot \sum_{i=1, i \ne j}^{S} \int_{E_{ij}} p(x \mid H_j) dx = \sum_{j=1}^{S} p(H_j) \cdot \sum_{i=1, i \ne j}^{S} p(x \in E_{ij} \mid H_j). \tag{4.61}$$

In reality, at validity of hypothesis H_j decision is accepted $(S-1)$ times when hypotheses H_j and H_i, $i = 1,...,S$, $i \ne j$, are compared two by two. Every time the probability of acceptance of the wrong decision at validity of hypothesis H_j, i.e. the probability of passing of the correct decision is equal to $P(x \in E_{ij} \mid H_j)$. Therefore total probability of acceptance of other hypotheses at validity H_j, i.e. the risk is equal to

$$\sum_{i=1, i \ne j}^{S} P(x \in E_{ij} \mid H_j).$$

It is not difficult to calculate

$$P(x \in E_{ij} \mid H_j) = P\left(\sum_{\ell=1}^{m} \frac{a_\ell^j - a_\ell^i}{\sigma_\ell^2} x_\ell \le \tilde{\lambda}_{ij} \mid H_j \right) = \Phi\left(\Phi^{-1}(\beta) - \sqrt{\sum_{\ell=1}^{m} \frac{(a_\ell^j - a_\ell^i)^2}{\sigma_\ell^2}} \right),$$

where Φ is standard normal function of probability distribution.

If we shall designate

$$G_{ij} = \sum_{\ell=1}^{m} \frac{(a_\ell^j - a_\ell^i)^2}{\sigma_\ell^2},$$

then, finally, for average risk we have

$$r(\delta)=\sum_{j=1}^{S}P(H_j)\cdot\sum_{i=1,i\neq j}^{S}\Phi\left(\Phi^{-1}(\beta)-\sqrt{G_{ij}}\right).$$

When the number of hypotheses is equal to two, i.e. $S=2$, the quasi-optimal algorithm turns to the optimum. Thus, for two hypotheses the optimum decision is accepted analytically.

4.8. Ratio of Values of the Risk-Functions in Put Problems and Their Numerical Researches

Analysis of relations of mean risk values corresponding to the stated conditional Bayesian problems is given in [133]. It is shown there that the mean risk value calculated for problem with restrictions (4.16) is always greater than the mean risk value calculated at restrictions (4.13), and the mean risk value at restrictions (4.10) is between the previous two values. The mean risk value calculated at restrictions (4.18) is always not greater than the mean risk values at restrictions (4.16).

It is a fact that the mean risk value in unconstrained problem of many hypotheses testing is always lesser than the mean risk value calculated in conditional problems, and the mean risk value corresponding to quasi-optimal rule of hypotheses testing is always not less than the mean risk values corresponding to conditional Bayesian problems. This fact is a consequence of rigidity of restrictions corresponding to these problems. Really, $\beta>1-\alpha$ at number of hypotheses $S>2$, and for unconditional problems there are no restrictions at all. To demonstrate this fact, relations of mean risk values calculated for unconditional, conditional and quasi-optimal problems of hypotheses testing, depending on information distance between tested hypotheses, are shown in Figure 4.2. The problem with restrictions (4.13) is taken as unconditional Bayesian problem, since the minimum mean risk value among all the conditional Bayesian problems corresponds to it.

To illustrate the above-stated, the following simple example is taken: the number of hypotheses $S=5$; dimensionality of parametric space $m=2$; coordinates of hypothetical points in initial state - $a_1(1;1)$, $a_2(2;1)$, $a_3(3;2)$, $a_4(4;1)$, $a_5(3;3)$; variances of measured parameters σ_1^2=0.5, σ_2^2=0.5; coordinates of the measurement result *x*(2.7; 2.3); *a priori* probabilities $p(H_i)=0.2$, $i=1,...,5$.

In all the cases, by all decision rules, hypothesis H_3 was accepted, which corresponds to reality. In Figure 4.2, r_{unc}, r_c and r_q denote mean risk values in unconditional, conditional and quasi-optimal problems of hypotheses testing, correspondingly. The first point on axis of abscissas corresponds to initial values of hypothetical points, the second point corresponds to the changed coordinates of the fifth hypothetical point a_5 (5; 4); to the third point, correspond

the changed second and fifth hypothetical points $a_2(2;\ 4)$, a_5 (5; 4); to the fourth point - changed hypothetical points $a_2(2;\ 4)$, $a_4(6;\ 1)$, $a_5(5;\ 4)$; to the fifth point - changed hypothetical points $a_2(2;\ 4)$, $a_4(6;\ 1)$, $a_5(5;\ 6)$.

Figures 4.3 and 4.4 show the mean risk of unconditional tasks plotted against the variance of measured parameters and the information distance between hypotheses, correspondingly. Calculations were made for the above given example. The figures illustrate the logical dependence of mean risk of variance of parameters and the information distance between hypotheses and confirm the fact of dependence of mean risk values, i.e. of quality of made decisions, on valid choice of penalty function. At differential choice of penalty function, mean risk value considerably diminishes as compared with the step loss function, when the price of any error is one and the same and doesn't depend on the extent of its roughness.

Let us give some results of the developed algorithms testing for conditional Bayesian rules. Calculations were made for the above given example. Figures 4.5-4.7 show dependencies of the risk function on: variance of measured parameters; information distance between tested hypotheses and probability of correct expecting of hypotheses, correspondingly. The figures illustrate the logical dependencies of the risk function on these parameters, i.e. the risk function increases with increasing of the variance of measured parameters, the risk function decreases with increasing of the information distance between tested hypotheses and the risk function, i.e. averaged probability of true decisions rejection, increases with increasing of the probability of making true decisions.

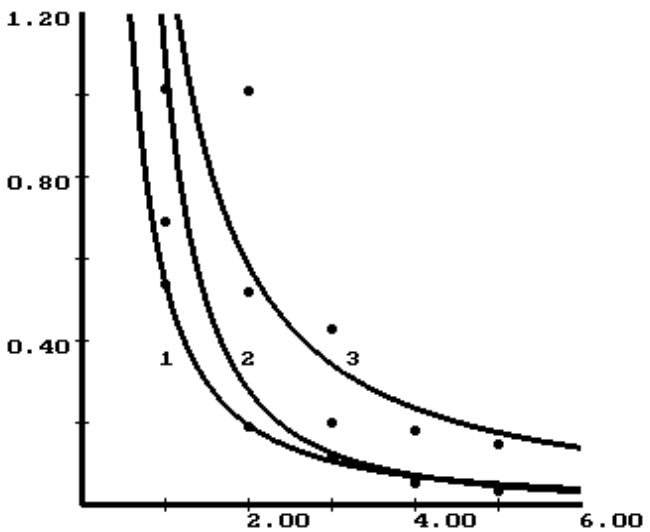


Figure 4.2. Mean risk values versus information distance between hypotheses: (1) $100 \cdot r_{unc}$; 2) r_c; (3) r_q.

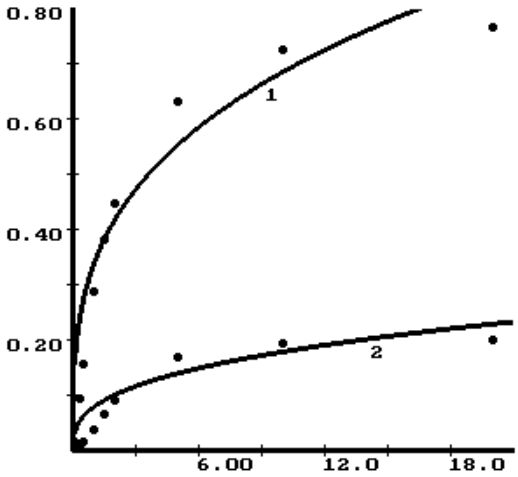


Figure 4.3. Risk function versus the variance of measured parameters (1) r_{st}; (2) $10 \cdot r_{nst}$.

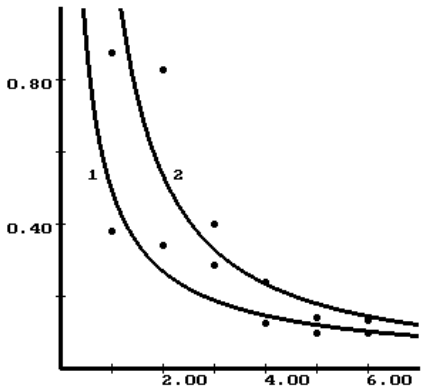


Figure 4.4. Risk function versus the information distance between hypotheses (1) r_{st}; 2) $100 \cdot r_{nst}$.

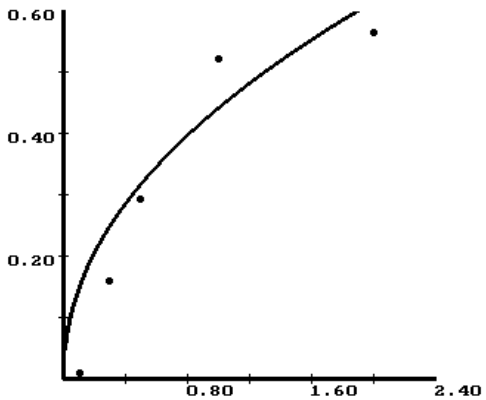


Figure 4.5. Risk function r versus the variance of measured parameters.

Should be noted the following fact: $\sigma^2 = 1$ and 2; it is not available that the power of criterion $(1-\alpha) = 0.95$ because of effect shown on the Figure 4.1. In these cases $(1-\alpha) = 0.92$ at $\sigma^2 = 1$ and $(1-\alpha) = 0.98$ at $\sigma^2 = 2$ (see Figure 4.5).

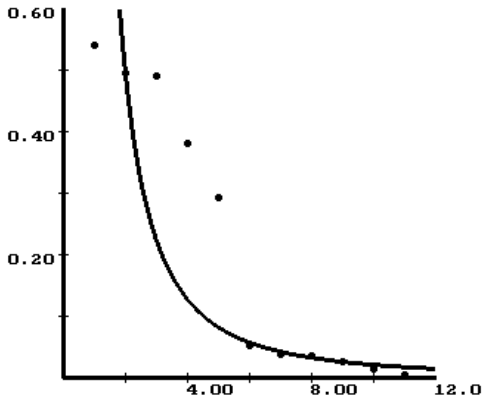


Figure 4.6. Risk function r versus information distance between tested hypotheses.

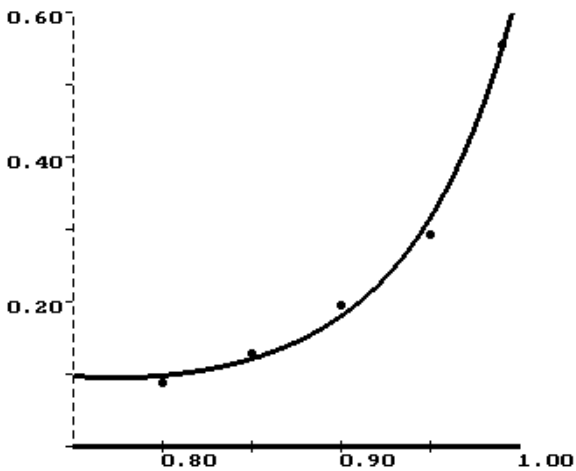


Figure 4.7. Risk function r versus probability of making true decisions.

4.9. CONCLUSIVE REMARKS

This chapter is dedicated to a problem of acceptance of the statistical decisions by results of experiment, founded on one of the classic approaches - the Bayesian approach. In it is used as the classical Bayesian formulation of a test of hypothesis encompassing by definition of the decision rule with the help of unconditional minimization of a risk function, so the new approach encompassing by definition of the decision rule by the solution of a problem of constrained optimization of a risk function at miscellaneous limitations on probability of acceptance of the incorrect solutions concerning the verity of hypothetical values of distribution parameters. The generalization of classical Bayesian formulation of test of many

hypotheses encompassing that the dimension of the decision rule and quantity of tested hypotheses do not coincide is made. In the given statement the solutions are born more differentiated, concerning not of hypotheses as a whole, but of each tested parameter. The classical Bayesian statement is a particular case of such statement, as at not intersected hypotheses, i.e. in a case, then they do not contain common parameters, the above-mentioned statement coincides with classical statement. Besides in the chapter are given the quasi-optimum rule of test of many hypotheses. Are determined the optimum decision rules in all put problems of test of many hypotheses for a density of distribution of probability of a general view. These decision rules are rendered concrete up to working formulas and algorithms for such relevant distribution from the application of probability theory and mathematical statistics, what the normal distribution of probabilities is. At development of these algorithms some problems having independent concern are resolved. Such, as calculus of a multidimensional normal integral on area of the composite configuration by approximating these areas or by decomposing integrand density by the way of series, decreasing of dimension of a multidimensional normal integral without a loss of information. The outcomes of an experimental research of designed algorithms are adduced.

The solution of many practical problems from miscellaneous areas of science and engineering under the contents and the object in views demand the approach, the essence which one is encompass in usage of the above-stated decision rules of test of many statistical hypotheses. For illustration we shall bring below some examples of technical problems at the solution which one will be used in the given chapter obtained outcomes.

For control of condition of environmental objects, there are created the automated controlling systems, consisting from analyzers automatically measuring controlled parameters of an environment and transmitting their values to the Control Station by communication channels, where on the basis of processing of this information on the computer, the solutions on a condition of controlled object are born [1]. The problem of control of condition of an environment includes a problem of identification of emergency pollution sources for taking a step on their elimination. For the solution of this problem in question of making the decision there is used the above-stated algorithms which are realized in software “Identification of River Water Pollution Sources by Means of Automated Control Systems” developed for IBM-compatible computers in the project G-047 of ISTC (International Science and Technology Center) (1998-2000) (see Chapters 5 and 7). The conditional approach of test of many hypotheses was utilized with the purpose of restriction of probability incorrectly accused in pollution of pollution sources, at minimization of probability of non-detection of the true initiators of pollution.

Designed rules of test of many hypotheses also can be successfully applied at problem solving of detection and tracking of objects, driving in space, on the basis of the radar measuring information [133, 186]. At detection it is required to minimize a probability of incorrectly detected objects at restrictions on probability of the failed true objects.

Above offered algorithms also can be used in seismology for solution of a problem of detection of geomagnetic surges stimulus source by results of measurement of several seismological stations. Also can be successfully used in pharmacology at manufacturing of poison keeping drugs for minimization of probability of no dosage at limitations of an over dosage especially dangerous for health of the people of components.

Chapter 5

MATHEMATICAL BASES FOR SOLVING PROBLEM OF IDENTIFICATION OF THE SOURCES OF EXCESSIVE RIVER POLLUTION

5.1. ESSENCE OF IDENTIFICATION PROBLEM

One of the actual tasks of environmental condition monitoring problem is that of identification of the emergency release sources to take measures on their elimination. This task is especially actual for city conditions, because the large number of pollution sources doesn't allow to control each of them. The solution of this task has not only an ecological, but a significant economical effect as well, which is reached by means of minimization of technical faculities, in particular, the measurement facilities needed for the stand-alone control of each pollution source. This task is also actual for large factories and plants with biochemical purification of waste water in order to identify those sections of shops which are guilty of waste water pollution over the norm (see section 3.6) [1, 179, 187].

In spite of such actuality this task is not solved in general form till present and previous works of the authors, though a lot of authors note its great importance for solving the problem of monitoring of the pollution of environmental water objects [189, 192-197]. In this chapter are described algorithms, developed by authors, for identification of emergency pollution sources in rivers between two controlled ranges by means of automated systems [180, 182, 188, 180]. In chapter 7 is described the software of realization of these algorithms for IBM-compatible computers [93, 94].

The developed program package for identification of emergency release sources may be included into any available or newly developed automated system for control of water object pollution level. The system is shown on Figure 5.1 as an illustration diagram. Some of developed under the guidance of one of the authors of this work the automated systems are described in [1]. The number and the types of water objects, for which the developed program package may be used, are limited by the mathematical models of pollutants transfer, included into the library of the developed package. The library is of open type, i.e. newly developed models may be included into it and thus the list of water objects for which this package is suitable can be expanded.

5.2. FORMALIZATION OF THE PROBLEM

Let's consider the problem of identification of the river water pollution sources located between two controlled ranges by means of automated systems [1, 187]. The proposed algorithms are built with the assumption that the pollution sources have either different composition of waste water or (at the same composition) different ratios of ingredients.

Let the river water condition be controlled by M automated stations on the section under consideration. Each of the stations controls m physical–chemical parameters. Let's denote the water quality index at the j-th station, i.e. in the j-th controlled range of the river at t_N moment, by $\hat{X}_j(t_N) = \{\hat{x}_{jp}(t_N)\}$, $j = 1,...,M$; $p = 1,...,m$.

The symbol over X indicates that not exact values of the controlled parameters but their estimations are known in the j-th range.

Let pollution have place at t_N moment in the j-th range, i.e.

$$\hat{X}_j(t_N) = \{\hat{x}_{jp}(t_N)\} \in \overline{\Gamma},$$

where $\overline{\Gamma}_j = X - \Gamma_j$; X – m-dimensional parametric space; Γ_j – m-dimensional region of the unpolluted water in the j-th range,

$$\Gamma_j = \left\{\hat{x}_{jp}(t): \ \mu_{jp}^1 < \hat{x}_{jp}(t) \le \mu_{jp}^2; \ \ \forall p : p \in (1,...,m)\right\};$$

$(\mu_{jp}^1, \mu_{jp}^2]$ – region of the unpolluted by parameter p water in the j-th range.

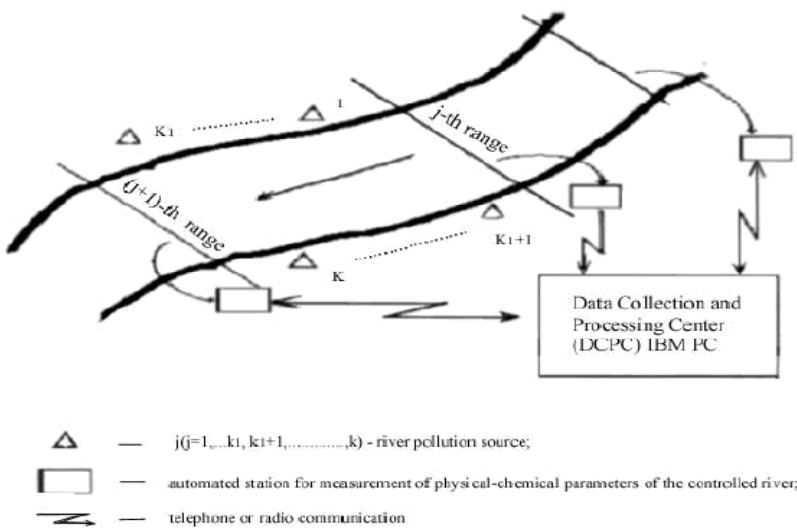


Figure 5.1. Conventional scheme of the automated system for control of river pollution level.

In formation of water quality in the j-th range $\hat{X}_j(t_N)$ are the following participants: the $(j-1)$-th range, $\hat{X}_{j-1}(t_N-\tau_{j-1})$, where τ_{j-1} is the time for water to run from the $(j-1)$-th range to the j-th one; K – controlled objects with the known concentrations of the substances being released $Z_{j-1,k}(t_N-\tau_k)$, $k=1,...,K$, where τ_k is the time for water to run from the k-th controlled object to the j-th range; R – uncontrolled objects, which in the normal mode of operation release concentrations $Y_{j-1,r}(t_N-\tau_r)$, $r=1,...,R$, and in the emergency mode may have additional releases $\Delta Y_{j-1,r}(t_N-\tau_r)$, $r=1,...,R$, where τ_r is the time for water to run from the r-th uncontrolled object to the j-th range. Other uncontrolled factors are called "noise". Let's denote their influence on the quality of water in the j-th range by $\overline{X}_0^j(t)=\{\overline{x}_{0p}^j(t)\}$, $p=1,...,m$.

After introducing of denotations the model of water quality formation in the j-th range assumes the following form

$$\hat{X}_j(t_N)=F_j[\hat{X}_{j-1}(t_N-\tau_{j-1}),\ \lambda_{j-1};Z_{j-1,k}(t_N-\tau_k),\ \alpha_{j-1,k}\ (k=1,...,K);$$
$$Y_{j-1,r}(t_N-\tau_r),\ \beta_{j-1,r}\ (r=1,...,R)]+\overline{X}_0^j(t_N), \qquad (5.1)$$

where F_j is the known operator corresponding to the process of formation of water quality in the j-th range; τ, λ, α and β are parameters characterizing the time of running to the j-th range and the peculiarities of formation of water quality in it.

If there is a pollution, i.e. when $\hat{X}_j(t_N)\in\overline{\Gamma}$, the model of water quality formation takes on the following form

$$\hat{X}_j(t_N)=F_j[\hat{X}_{j-1}(t_N-\tau_{j-1}),\ \lambda_{j-1};Z_{j-1,k}(t_N-\tau_k),\ \alpha_{j-1,k}\ (k=1,...,K);$$
$$Y_{j-1,r_1}(t_N-\tau_{r_1}),\ \beta_{j-1,r_1}\ (r_1\in R');$$
$$Y_{j-1,r_2}+\Delta Y_{j-1,r_2},\ \beta_{j-1,r_2}\ (r_2\in R'')]+\overline{X}_0^j(t_N) \qquad (5.2)$$

where $R'\bigcup R''=R$, $R'\bigcap R''=0$, and the division of set R into subsets R' and R'' being unknown.

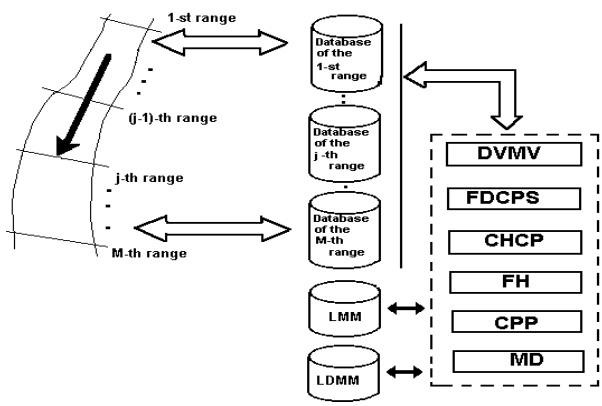
The task consists in dividing of set R into subsets R' and R'' at the moment of pollution detection. Upon detection of pollution in the j-th range by means of operator F_j from (5.2), the concentrations in the j-th range are determined with the assumption that the emergency release was made by one or two, etc., or r uncontrolled objects, i.e. there are calculated m-dimensional points $X_j^{i_1,...,i_r}(t_N)$, where $i_j\in(1,...,R)$; $i_{j_1}\neq i_{j_2}$; r indicates

the number of uncontrolled objects, which are suspected in the simultaneous emergency release. The number of points $X_j^{i_1,\ldots,i_r}(t_N)$ for each population r out of R objects is equal to C_R^r ,and the total number of all the points is $\sum_{r=1}^{R} C_R^r = 2^R - 1$. It is necessary to decide which population r of uncontrolled objects made the emergency release, i.e. it is necessary to test hypotheses

$$H_i : M\left(\hat{X}_j(t_N)\right) = X_j^{i_1,\ldots,i_r}(t_N), \quad i = 1,2,\ldots,2^R - 1. \tag{5.3}$$

5.3. GENERALIZED BLOCK-DIAGRAM FOR SOLVING IDENTIFICATION PROBLEM

For visualization of inter-consistency and sequence of fulfillment of separate problems in Fig. 5.2 is given the generalized block diagram of solving the problem of identification of emergency release sources. The arrows indicate the execution sequence of programs for the marked problems and the directions of information flows. To realize the problem of identification of emergency release sources it is necessary to solve, in accordance with the sequence indicated by the arrows in Figure 5.2, the following tasks: decorrelation of the vector of measured values (DVMV); formation of different combinations of pollution sources (FDCPS); calculation of hypothetical concentrations of pollutants in the lower controlled range according to mathematical models (CHCP); formation of hypotheses concerning emergency pollution sources (FH); calculation of a prior probabilities of the formed hypotheses (CPP); making a decision on the guiltiness of sources in the emergency pollution (MD).



LMM - library of mathematical models of pollutants transfer in rivers;
LDMM - library of methods of making decision;
$\Rightarrow$ - direction of information flow;
$\longrightarrow$ - direction of execution sequence of problems.

Figure 5.2. Generalized block-diagram for solving the problem of identification of emergency release sources.

In the library of mathematical models described the processes of the transport of pollution substances in rivers there are realized mathematical models and algorithms of their calculation described in Chapters 1 and 2, and in the library of the methods of making a decision concerning guilty in emergency dropping there are realized Bayesian methods and algorithms of testing many hypotheses described in Chapter 4. For simplification of the procedure of making decision there are described algorithms of cluster-analysis in section 5.6.

5.4. ALGORITHM OF HYPOTHESES FORMATION

The total number of m-dimensional points, which suppose different combinations of uncontrolled objects to be emergency release sources, at exhaustive search of all possible variants, is $2^R - 1$, where m is the number of parameters being measured, R – the number of uncontrolled objects. For real values of m and R, to perform necessary computations for such a number of variants within practically acceptable period of time is impossible, even on modern powerful personal computers. It is necessary to develop an algorithm, allowing a significant reduction in the amount of searching of different combinations of uncontrolled objects, but still providing that the remained combinations would include the true combinations of uncontrolled objects. The algorithm given below allows to reduce significantly the exhaustive search of necessary variants and to solve the problem of identification of the sources of excessive pollution within practically acceptable period of time.

Let the i-th uncontrolled object release some m_i parameters out of m parameters controlled by the analyzer in the j–th range. Let pollution by some $n \le m$ parameters be registered in the j–th range at t_N moment. Then, from the total number of uncontrolled objects R, are chosen only those objects $R_1 \le R$, which release n parameters.

Let $\left(x_{i_1},...,x_{i_{n_i}}\right)$ denote the set of parameters released by the i-th uncontrolled object, $n_i \le m$, $i = 1,...,R$; $\left(x_{i_1},...,x_{i_{n_i}}\right)$ – the parameters exceeding the allowable limit of concentration (ALC) in the j–th range. Then, only those objects, for which $\left(x_{i_1},...,x_{i_{n_i}}\right)\bigcap\left(x_{j_1},...,x_{j_n}\right) \neq \varnothing$ will remain as suspected in the emergency release. Let's denote the number of such objects by $R_1 \le R$.

Only n parameters exceeding the allowable limit of concentration will be used for making decision on pollution sources, as the other parameters will be non-informative for the problem under consideration.

Thus, the number of parameters is reduced to n_1, and the number of the objects suspected in emergency release – to R_1.

Only concentrations of n_1 parameters are calculated according to the developed models. The parameters are calculated independently.

Let's consider one parameter $x_{j_1} \in (x_{i_1},\dots,x_{i_n})$. Let $R_2 \le R_1$ uncontrolled objects take part in formation of x_{j_1} parameter. We are modeling the value of x_{j_1} parameter in the j–th range on the assumption that the release was made by some one uncontrolled object out of R_2 uncontrolled objects, by some two, three and so on uncontrolled objects, and the corresponding distances $d_{i_1,\dots,i_r} = d(\hat{x}_{j_1}, x_{j_1})$ are being calculated. For each r value, i.e. for each population of uncontrolled objects, the minimum value $d^*_{i_1,\dots,i_r} = \min d_{i_1,\dots,i_r}$ is being calculated. The confidence interval around $\hat{x}_{j_1}$ point, i.e. $[\hat{x}_{j_1} - t_\alpha \cdot \sigma_{\hat{x}_{j_1}}, \hat{x}_{j_1} + t_\alpha \cdot \sigma_{\hat{x}_{j_1}}]$ is being formed. If some successive value from sequence $d^*_{i_1}, d^*_{i_1,i_2},\dots,d^*_{i_1,\dots,i_r},\dots$ falls outside the confidence interval and the preceding value is within the confidence interval, the calculation is stopped, and those objects out of R_2, for which the corresponding distances d^* have fallen within the confidence interval, are included into the suspected set of emergency pollution sources. Let's denote their set by R'_2. (Concentrations x_{j_1} for objects from R'_2 are already calculated and will be used later when forming multidimensional points). These objects subtract from the set R_1. We'll receive $R_{1,2} = R_1 - R'_2$ – the set of uncontrolled objects for further consideration.

Let's consider the second parameter $x_{j_2} \in (x_{j_1},\dots,x_{j_n})$. Let $R_3 \le R_1$ uncontrolled objects take part in formation of x_{j_2} parameter. We are modeling the value of x_{j_2} parameter in the j–th range on the assumption that the release was made by some one uncontrolled object out of R_3 uncontrolled objects, by some two, three and so on uncontrolled objects, and distances $d_{i_1,\dots,i_r} = d(\hat{x}_{j_2}, x_{i_2})$ are being calculated. For each r value, i.e. for each population of uncontrolled objects, the minimum value $d^*_{i_1,\dots,i_r} = \min d_{i_1,\dots,i_r}$ is being calculated. The confidence interval $[\hat{x}_{j_2} - t_\alpha \cdot \sigma_{\hat{x}_{j_2}}, \hat{x}_{j_2} + t_\alpha \cdot \sigma_{\hat{x}_{j_2}}]$ is being formed. If some successive value from sequence $d^*_{i_1}, d^*_{i_1,i_2},\dots,d^*_{i_1,\dots,i_r},\dots$, falls outside the confidence interval and the preceding value is within the confidence interval, the calculation is stopped, and those objects out of R_3, for which the corresponding distances d^* have fallen within the confidence interval, are included into the suspected set of emergency pollution sources. Let's denote their set by R'_3. They are subtracted from $R_{1,2}$.

We'll receive $R_{1,3} = R_{1,2} - R_3'$ - the set of uncontrolled objects for further consideration.

Then the third parameter x_{j_3} is taken into consideration and so on, until set $R_{1,k}$, $k \in (1,...,n)$ is an empty set.

Those S populations of uncontrolled objects, which fell into this set while considering separate parameters, will remain being suspected in pollution. Concentrations of those parameters out of m, which were not calculated when considering separate parameters, must be calculated for each population. The received m-dimensional points will constitute S hypotheses, which must be tested for making the final decision.

5.5. CALCULATION OF A PRIOR PROBABILITIES

A certain a prior probability, depending of its hypothetical participation in emergency pollution, is assigned to each uncontrolled object so as to hold

$$\sum_{i=1}^{R} P(ob_i) = 1 \quad .$$

If the objects have several emergency modes, each emergency mode will be recognized as a new object. Thus, the total number of uncontrolled objects R will be equal to the number of all emergency modes of the uncontrolled pollution sources.

After formation of hypotheses concerning guiltiness of sources of the emergency pollution, i.e. after defining the set of points of mathematical expectation of measurement vector, the a prior probabilities of hypotheses, corresponding to the chosen points of mathematical expectation, are found in the following way.

Let's assume that mathematical expectation a_i, $i = 1,...,S$, was calculated with the assumption that objects $ob_{j_1}, ob_{j_2},..., ob_{j_{K_i}}$, are guilty. Then

$$Q(a_i) = \frac{1}{K_i} \sum_{l=1}^{K_i} P(ob_{j_l})$$

and

$$p(a_i) \equiv p(H_i) = \frac{Q(a_i)}{\sum_{i=1}^{S} Q(a_i)}, \quad i = 1,...,S \quad .$$

5.6. DECORRELATION OF THE MEASURED VALUES VECTOR

According to the note made in paragraph 4.1, preliminary decorrelation of a vector of the measured values does not influence results of testing hypotheses. As components of a vector of the measured values of controllable components of river water, generally, are correlated, for direct use in Chapter 4 given algorithms in the process of making decisions concerning guilt in emergency pollution, there is preliminary carried out decorrelation of a vector of measurements [126, 133, 191].

Let $x = (x_1,...,x_n)$ be m-dimensional normally distributed random vector with mathematical expectation $\mu = (\mu_1,...,\mu_m)$ and covariant matrix $W_{m\times m}$, i.e.

$$p_x(x) = (2\pi)^{-m/2} \left|W\right|^{-1/2} \exp\left\{-\frac{1}{2}(x-\mu)^T\ W^{-1}\ (x-\mu)\right\}. \tag{5.4}$$

For convenience of representation, let's denote $Y = x - \mu$, $W^{-1} = V = \left\|V_{ij}\right\|_{m\times m}$. Then

$$(x-\mu)^T\ W^{-1}\ (x-\mu) = Y^T\ V\ Y = A(Y;Y). \tag{5.5}$$

Let's introduce such orthogonal matrix $\alpha = \left\|\alpha_{ij}\right\|_{m\times m}$, the columns of which are eigenvectors of matrix V. Then

$$\alpha^T \cdot V \cdot \alpha = K = \begin{Vmatrix} K_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & K_{mm} \end{Vmatrix},$$

where K_{ii}, $i = 1,...,m$ is the i-th eigenvalue of matrix V.

Let's denote

$$(x-\mu) = \alpha\ \cdot K_1^{-1} \cdot Z,$$

where

$$K_1 = \begin{Vmatrix} \sqrt{K_{11}} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sqrt{K_{mm}} \end{Vmatrix}.$$

Then

$$Z = K_1\ \alpha^{-1}\ (x-\mu) = K_1\ \alpha^T\ (x-\mu). \tag{5.6}$$

With the new notations, quadratic form (5.5) may be rewritten as:

$$A(Y;Y) = Z^T (K_1^{-1})^T \alpha^T V \alpha K_1^{-1} Z = Z^T K_1^{-1} K K_1^{-1} Z = Z^T Z .$$

Since α and K_1 are, correspondingly, matrices of eigenvectors and eigenvalues of matrix V, Jacobian of such transformation is equal to $(\det W)^{1/2}$. With the new notations, probability density (5.4) may be rewritten as

$$p_z(Z) = (2\pi)^{-\frac{m}{2}} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m} Z_i^2\right\}.$$

Thus, we have received that vector

$$Y = K_1\ \alpha^T\ x, \tag{5.7}$$

is normally distributed random vector with mathematical expectation μ and covariance matrix W.

5.7. ALGORITHMS OF CLUSTER-ANALYSIS FOR IDENTIFICATION OF EMERGENCY RELEASE SOURCES

Depending on the available a priori information it is possible to consider different procedures of testing hypotheses (5.3). In process of increase of a priori information there is possible to use more complex procedures of making decision providing higher reliability (see Chapter 4). In those cases when a priori information is unknown or the probability distribution law of the vector of measured parameters $\hat{x}(t_N)$ is unknown or when operative obtaining the decision even lower reliability is necessary, the procedure of making the decision is based on the distance between points $\hat{x}_j(t_N)$ and $\hat{x}_j^{i_1,\ldots,i_r}(t_N)$ (see section 5.2):

$$d_{i_1,\ldots,i_r} = d\left(\hat{x}_j(t_N), x_j^{i_1,\ldots,i_r}(t_N)\right).$$

That uncontrolled objects or populations of uncontrolled objects to which corresponds the minimum distance d, is considered to be the pollution source. Algorithms making decision based on the distance d refer to the algorithms of cluster analysis. In case, when, during the emergency release, one and the same object may release different concentrations, they should

be considered as releases from different uncontrolled objects, and the algorithms making decisions should be used.

Depending on the chosen measure of the distance d there is a large number of the algorithms of cluster analysis [see, for example, 198 – 200, 201 – 209].

Two simple algorithms of cluster analysis are given below based on the distances of Euclid and Makhalanobis. They are realized by authors in the package of identification of emergency pollution sources of rivers (see Chapter 7) side by side with Bayesian algorithms described in Chapter 4 [182, 187, 188].

Veracity of the decision made in this algorithm depends on the noise level $\bar{x}_0(t)$ (see section 5.2). With increasing of ratio $M\left(\hat{x}_j(t_N)\right)/\sqrt{D\left(\bar{x}_0^j(t)\right)}$, where M and D are signs of mathematical expectation and variance correspondingly, the probability of incorrect identification of pollution sources decreases.

In the absence of covariant matrix of the measurement vector $\hat{x}(t_N)$, the Euclidean distance is used as a distance measure

$$d_{i_1,\ldots,i_r} = \left(\hat{x}_j(t_N) - x_j^{i_1,\ldots,i_r}(t_N)\right)^T \left(\hat{x}_j(t_N) - x_j^{i_1,\ldots,i_r}(t_N)\right).$$

If water condition in the j–th range is controlled by the automated station, by means of which covariant matrix W_j is estimated on the base of accumulated measurement information $\hat{x}_j(t_N)$, $N = 1,2,\ldots$, then the Makhalanobis distance is used as a distance measure:

$$d_{i_1,\ldots,i_r} = \left(\hat{x}_j(t_N) - x_j^{i_1,\ldots,i_r}(t_N)\right)^T W_j^{-1} \left(\hat{x}_j(t_N) - x_j^{i_1,\ldots,i_r}(t_N)\right).$$

The advantages of this method are: simplicity of its realization and minimum of a priori information needed. However, even if a priori information is available, it is impossible to use it in this case. All pollution sources in this procedure are equally dangerous. That is why it is preferable to use Bayesian algorithms of making decision, described in chapter 4, free of these disadvantages.

The described algorithms of the cluster analysis were used in the realized problem of identification of the shops guilty of emergency pollution of sewage of Odessa nitrogen factory in the computer-aided monitoring system of quality of sewage of this factory which has been developed and introduced at factory in 1985 – 1988 under the guidance of the authors of the given book. In the problem of identification as mathematical models (see paragraph 5.2) simulation models of formation of quality of sewage of this factory, described in paragraph 3.6, were used.

Chapter 6

SOFTWARE OF MATHEMATICAL MODELS OF POLLUTANTS TRANSPORT IN RIVERS

6.1. ASSIGNMENT AND POSSIBILITY OF THE PACKAGE

The description of the applied program package created by the authors for realization of mathematical models of pollutants transport in rivers is given in this Chapter [226]. It is designed an up-to-date as convenient reliable tool for experts in different fields of knowledge (biology, ichthyology, ecology, hydrology, building, agriculture etc.), allowing them to calculate the polluting substance concentrations at any point of the river depending on the quantity and the conditions of discharging from several pollution sources. As the mathematical models of water quality formation in the river under the influence of several pollution sources, spatially one-, two- and three-dimensional advective-diffusion models at different initial and boundary conditions (see Chapter 1) are realized in the package: a) an advective–diffusion equation with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self–purification of the river; b) an advective–diffusion equation with boundary condition of full mixing at the end of the controlled section; c) an advective–diffusion equation ignoring the vertical advection with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self –purification of the river; d) an advective–diffusion equation ignoring the vertical advection with boundary condition of full mixing at the end of the controlled section; e) a diffusion equation with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self–purification of the river; f) a diffusion equation with boundary condition of full mixing at the end of the river controlled section. For the abovementioned mathematical models, there are use computation schemes described in Chapter 2.

In the package there are the options of inputting and editing the initial data describing the geographical, geometrical and hydrological features of the simulated section of the river, the condition and the specific features of pollution of the river, the quantity and the name of the pollutant of interest, the types of used models and restrictions, the ways of assignment of these data etc. There are the options of choosing the language of dialogue with the package, the conditions of computation realization, the desirable accuracy of computation, the type and

format of output of the results. At any stage of working with the package, there is an option of help concerning the methods which are realized in the package, the capabilities and specific features of the package, the parameters of tasks and obtained results.

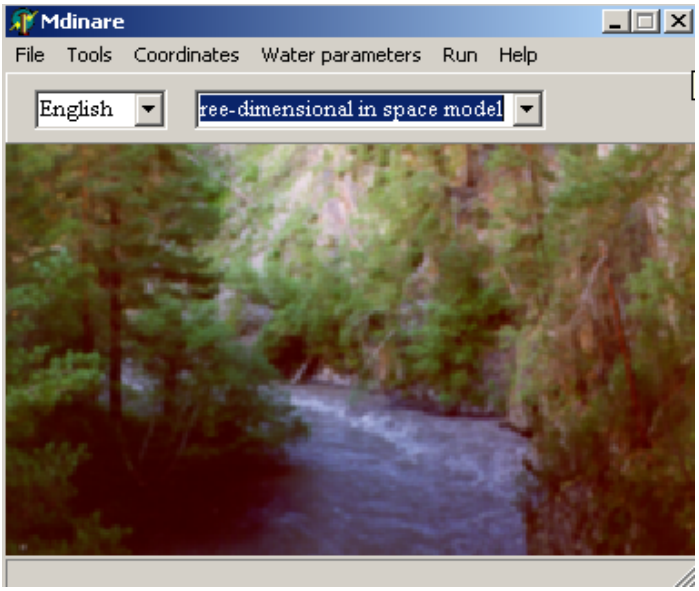


Figure 6.1. Sections of main menu of the package.

The choice of these possibilities is carried out by means of appropriate options from the commands of the main menu of the package. The main menu includes the following commands and options (see Figure 6.1): File (Page setup, Printer setup, Exit), Tools (Language, Model, Save options, Autosave), Coordinates (Type of coordinates, Banks and bottom, Flow velocity, List of objects, Objects, Convert files), Water parameters (List of substances, Upper cross-section, Capacities of sources, Coefficients of diffusion, Coefficient of non-conservatism, Coefficient of decreasing), Run (Accuracy, Calculations) and Help (Contents, Algorithms). The desirable language of dialogue with the package and the type of diffusion equation are selected directly from two pull-down lists. The description of purposes and capabilities of these options is given below.

6.2. Input and Editing of the Initial Data

The input of information necessary for operation of the package is performed in the form of separate constants, tables or the choice of the appropriate line from the pull-down. Let's adduce the substantial description of this information.

The data, which are not represented as tables. In the list given below, some parameters are common for all sections of the river, and some are specific for the chosen section; the latter are marked by the sign "d" in square brackets. The parameters marked by the sign "n" in square brackets are not saved in files.

- Type of model – one-dimensional, two-dimensional or three-dimensional. It is selected from the drop-down list displayed directly on the main toolbar or by selection of the option "**Model**" from the command "**Tools**" (see Figure 6.2).
- The indicator determining the method of the numerical solution of two-dimensional and three-dimensional diffusion equations – by means of iteration algorithm (see Item 1 of paragraph 2.1.2) or by representation of the sought-for solution as a linear combination of the solutions of one-dimensional equations (see Item 2 of the same paragraph) (see Figure 6.2).
- The number of sections of the river which can be considered in the package (see Figure 6.2).
- The number of polluting substances in the available list (see Figure 6.2).
- The indicator determining the type of coordinates (Cartesian or curvilinear), which are listed in the tables "Banks and bottom" and "Objects". It is switched by means of the option "Type of coordinates" (see Figure 6.3).

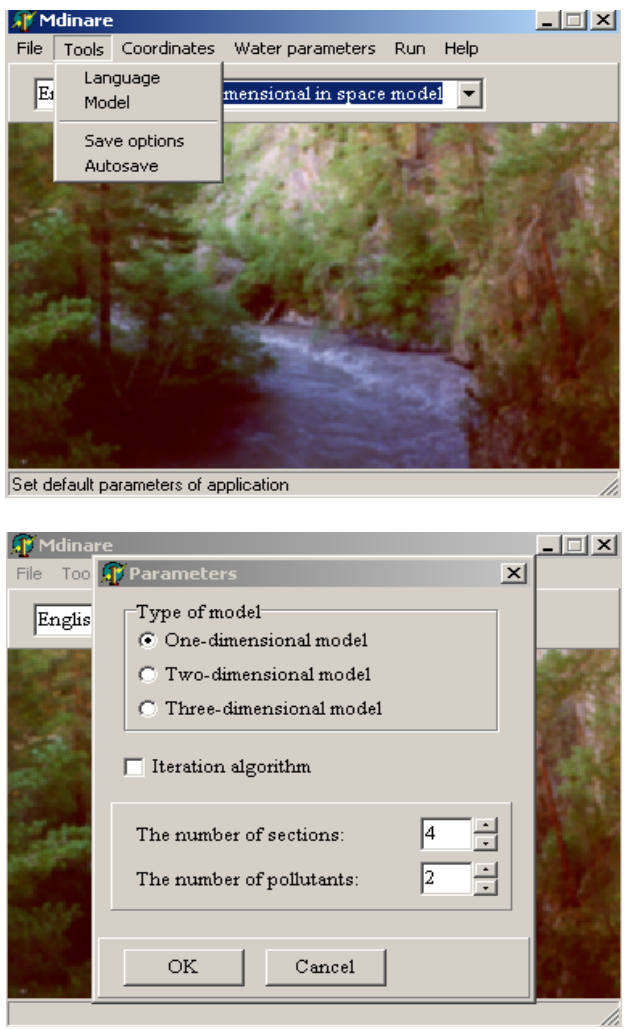


Figure 6.2.

- The parameters determining the accuracy of calculations at solving the diffusion equations. They include the total number of nodal points n, the number of nodal points n_2 along the axis Y (for the two-dimensional and three-dimensional models), the number of nodal points n_3 along the axis Z (for the three-dimensional model) and the factor c_t, determining the step of time discretization τ, i.e. the factor, which the value τ accepted by default is multiplied by. These parameters are entered by means of execution of the option "Accuracy" from the command "Run" of the menu of the main form (see Figure 6.4).

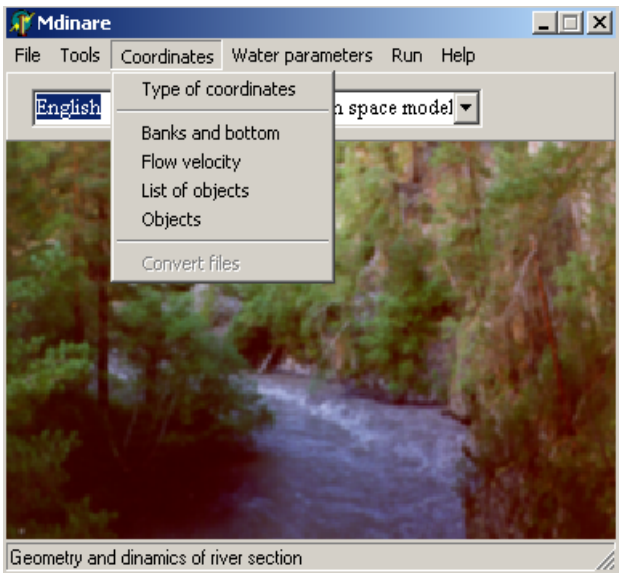


Figure 6.3.

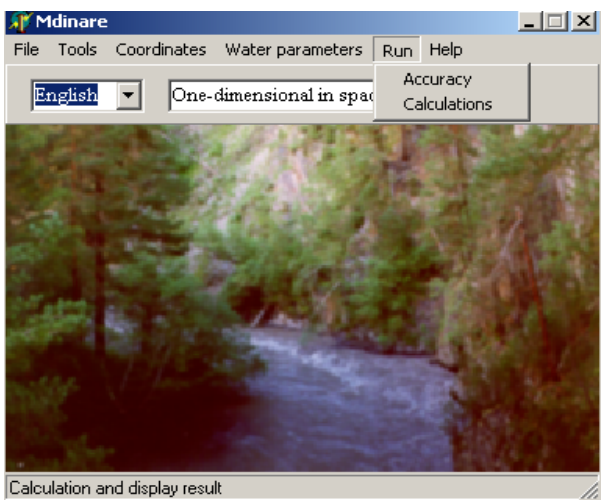


Figure 6.4.

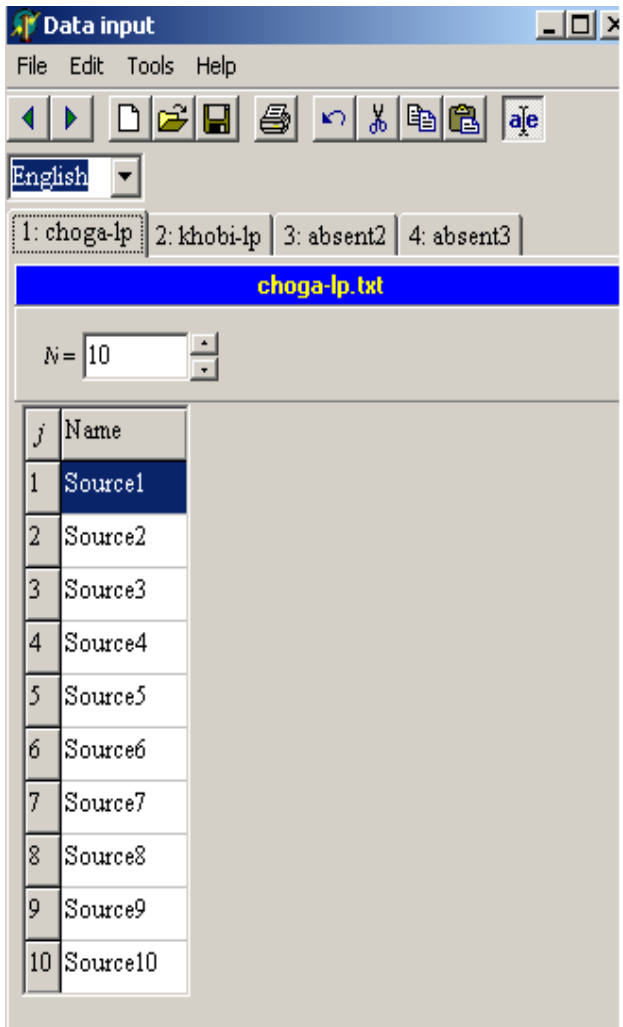


Figure 6.5.

- The number of the considered section. It is entered by execution of the option "Calculations" from the command "Run" of the menu of the main form (see Figure 6.4).
- The number of polluting sources within the considered section [d]. It is entered by means of the option "List of objects" from the command "Coordinates" of the menu of the main form (see Figure 6.3). The format of input is of the form shown in Figure 6.5.
- The indicator determining whether the diffusion equations for the considered section will be solved under non-classical boundary conditions (see Item 6 of paragraph 1.2) [d]. It is switched by means of the option "Calculations" from the command "Run" of menu of the main form (see Figure 6.4). The format of input is of the form shown in Figure 6.6.

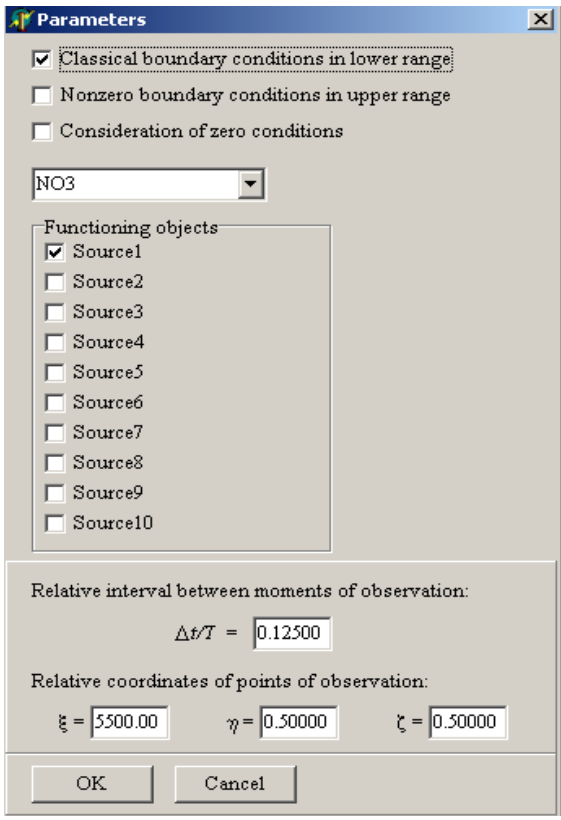


Figure 6.6.

- The indicator determining whether the given boundary conditions in the upper cross-section of the section will be taken into account at solving the diffusion equations or these boundary conditions will be taken equal to zero [d, n] (see Figure 6.6).
- The indicator determining whether the given initial conditions will be taken into account at solving of the diffusion equations or these initial conditions will be taken equal to zero [d, n] (see Figure 6.6).
- The polluting substance from the available list the concentration of which will be determined [d, n] (see Figure 6.6).
- The list of polluting sources which are considered to be operating at solving the diffusion equations. At solving of these equations, the capacities of other sources are considered equal to zero [d, n] (see Figure 6.6).
- The type of functions of spatial distribution of sources $D(u,x)$. This function can be trapezoidal, Gaussian or Loretzian (see paragraph 2.7).
- The type of function of discharge $A(v,x)$, determining the character of attenuation of capacities of the sources. This function can be stepwise, equal to the function of normal distribution or equal to the function of Cauchy distribution (see paragraph 2.7).

- Relative sizes of sources, i.e. the ratio between the parameter u and the spatial step used in the difference scheme grid along the corresponding coordinate axis (see paragraph 2.7).
- Relative duration of recession of the function of discharge, i.e. the ratio between the parameter v and the duration of operation of the source (see paragraph 2.7).

Below the number of polluting substances from the available list common for all sections is designated by M , and the number of polluting sources from the list corresponding to the considered section is designated by R .

The data given in the table "Banks and bottom" (Figure 6.3). Each of these parameters corresponds to some cross-section of the river with number j $(j = 1,..., N_h)$:

- ξ_j – the longitudinal coordinate;
- η_j – the cross coordinate of the point of the left bank;
- η'_j – the cross coordinate of the point of the right bank;
- x_j , y_j – the horizontal Cartesian coordinates of the point of the left bank;
- x'_j , y'_j – the horizontal Cartesian coordinates of the point of the right bank;
- h_{kj} $(k = 1,...,m_h)$ – the depth of the river at the point with cross coordinate $\eta_{kj} = \eta'_j + (\eta_j - \eta'_j) \cdot k / (m_h + 1)$.

Here N_h is the number of cross-sections; m_h is the number of equidistant points of the bottom in the cross-section. For each cross-section the value $w_j = \eta_j - \eta'_j$ represents the width of the river.

We have used the spline-interpolation for the functions $\eta_l(\xi)$ and $\eta_r(\xi)$, determining the cross coordinates of the points of bank lines of the river for the given ξ-coordinate, and the polynomial interpolation for the function $H(\xi,\eta)$, determining the depth of the river at the point with the given horizontal coordinates at the specified value of ξ.

Depending on the type of coordinates chosen by the user for data input – Cartesian or curvilinear, either the parameters x_j , y_j , x'_j , y'_j , h_{1j} , h_{2j} , … or the parameters ξ_j , η_j , η'_j , h_{1j} , h_{2j} , … are consistently entered in the columns of this table. The format of input of the latter is shown in Figure 6.7.

The data given in the table "Flow velocity" (Figure 6.3). The quantity v_j is the speed of the water flow in the cross-section with number j $(j = 1,..., N)$. The format of input is similar to the format of input of curvilinear coordinates.

The linear interpolation is used in the package to describe the dependence of the water rate $P(r) = E(r)\, v(r)$ on the ξ-coordinate.

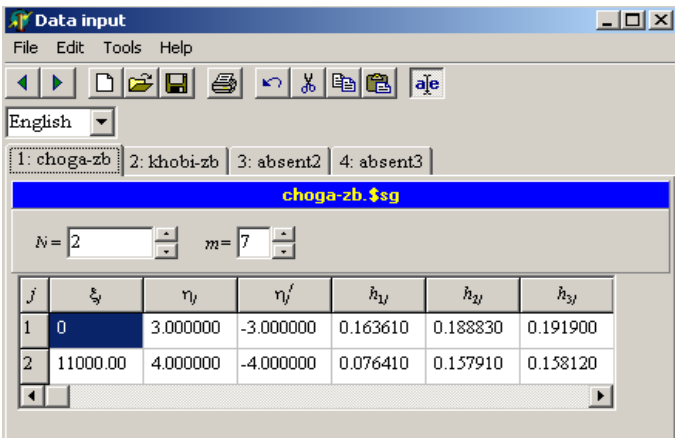


Figure 6.7.

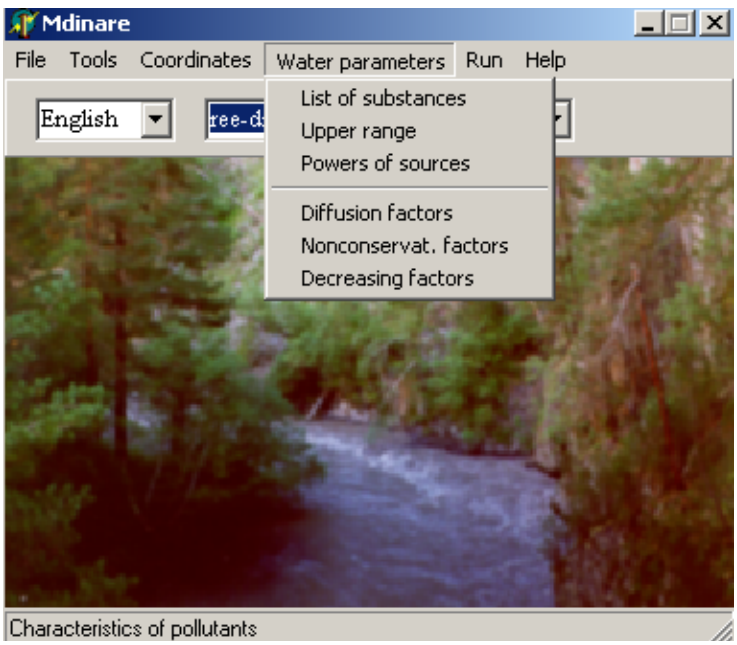


Figure 6.8.

The data given in the table "Objects" (Figure 6.3). Each of the following parameters corresponds to one of the pollution sources with number j $(j = 1,...,R)$.

- T_j is the duration of operation;
- ξ_j, η_j are the longitudinal and cross curvilinear coordinates;
- x_j, y_j are the horizontal Cartesian coordinates;
- z_j is the depth.

Depending on the type of coordinates chosen by the user for data input – Cartesian or curvilinear, the following parameters are consistently entered in columns of this table: T_j, x_j or ξ_j, y_j or η_j (for the two-dimensional and three-dimensional models), z_j (for the three-dimensional model). The format of input is similar to the format of input of curvilinear coordinates.

The data given in the table "The upper cross-section". The values σ_j are the boundary values of the polluting substance concentration with number j in the upper section $(j = 1,...,M)$.

They are entered by means of execution of the option "Upper range" from the command "Water parameters" of the menu of the main form (see Figure 6.8). The format of input is similar to the format of input of curvilinear coordinates.

The data given in the table "Capacity of sources" (Figure 6.8). The first column of the table contains the number of the source and its name; the second column contains water flow rate p_j of the j-th source of pollution; other columns contain concentration s_{jk} of polluting substances discharged into the river water by the j-th source; $j = 1,...,R$; $k = 1,...,M$. The format of input is similar to the format of input of curvilinear coordinates.

The data given in the tables "Coefficients of diffusion", "Coefficients of non-conservatism", "Coefficient of decreasing" (Figure 6.8). Each of the following parameters corresponds to one of the polluting substances with number j $(j = 1,...,M)$.

- K_x, K_y, K_z are the coefficients of turbulent diffusion in the upper cross-section;
- K'_x, K'_y, K'_z are the coefficients of turbulent diffusion in the lower cross-section;
- κ_j is the coefficient of non-conservatism in the upper cross-section;
- κ'_j is the coefficient of non-conservatism in the lower cross-section;
- l_j is the length of self-cleaning;
- q_j is the coefficient of self-cleaning.

The format of input is similar to the format of input of curvilinear coordinates.

The linear interpolation for dependence of parameters $K_x(r)$, $K_y(r)$, $K_z(r)$, $\kappa(r)$ on coordinate ξ is used in the package.

6.3. MANAGEMENT OF WORK OF THE SOFTWARE

6.3.1. Description of the Files used in the Software

Purpose of the basic files of the software. The enumerate below files are necessary for run and work of the software. Either these files or the folders specified before their names should be placed in one main directory (folder).

- **mdinare.exe** is the file running the software;
- **mdinare.num** and **mdinare.str** are the binary and text files containing parameters of work of the software which are read out at its running; both of this files change at performance of the command **Save options** or (in the case of switched on the option **Autosave**) at exit from the software (see 6.3.4); if these files are absent they are created automatically, thus values of parameters by default are established;
- **mdinare.dir** is the text file containing full names of data files which are automatically loaded into tables of data editing for each task at opening of corresponding forms (initial loading); in the case of switched on the option **Autosave** it changes at exit from the software; if this file is absent it is created;
- *.dic are the files-dictionaries serving for translation of text messages from English (see 6.3.2);
- ***.add** are the auxiliary files necessary for use of dictionaries; if they are absent they can be created at performance of the command **Language** from the main menu (see 6.3.2);
- ***.hlp** and ***.pdf** are the files containing the help information in different languages; the files **sample.hlp** and **sample.pdf** contain the help information in English;
- **mdinare.bmp** is the graphic file used by the software;
- **\Fonts\ *.ttf** are fonts used by the software; they are loaded into system at running of the software and unloaded at end of work of the software.

Syntax of used text files. The files **mdinare.str**, **mdinare.dir** and ***.dic** may be created or changed by means of any text editor. Thus these files delivered together with the software may be used as samples for their creation.

The file **mdinare.str** contains the following 3 lines (in view of the order of their arrangement in the file): 1) name of the chosen language (for example English, Russian, Georgian, etc.); 2) full name of working directory (for example C:\MSG\River\Data); 3) full name of the file running the program **Acrobat Reader** (for example C:\Program Files\Adobe\Acrobat5.0\Reader\Acro Rd32.exe).

Syntax of the file **mdinare.dir** is determined by the following rules:

- each line of this file contains names of the files concerning a specific target of input of initial data used in the software; it is necessary to watch not mixing numbers of lines in this file;
- if any line of this file contains a blank the part of this line following this blank is considered as a comment and is not used by the software;
- each line of this file or (at presence of a blank in it) the part of this line before the comment should contain one name of a file or several names of files separated by a semicolon "**;**", in the latter case different files concern to different editing windows on one form.

The files **mdinare.str** and **mdinare.dir** may be created or changed also during work of the software. Unlike them files-dictionaries ***.dic** may be created or changed only by means of a text editor.

Syntax of files-dictionaries is determined by the following rules: if M is the number of translated words and sentences then for each value $k = 0,...,M-1$:

- the line of this file with number $k+1$ contains a word or sentence in English which is necessary for translating;
- the line of this file with number $k+2$ contains the same word or sentence which was translated into chosen language;
- the line of this file with number $k+3$ is not used and may contain any comments.

Data files. Structure of a data file is determined by its extension in conformity with the following rules:

- First symbol of the extension always is '$';
- Second symbol of the extension is the first letter of name of type of the data which is written in the file; the letters 'b', 'i', 'w', 'l', 's', 'd' correspond to the types **byte**, **integer**, **word**, **longint**, **single**, **double**;

- Next symbols of extension determine the number N of columns of the table reserved for entered values; thus the real number of columns of the table which is visible on the screen at editing of data can be less N.
- If extension consists of three symbols then third symbol of extension is the letter of the Latin alphabet which serial number (beginning from 'a') is equal to the number N.
- If extension consists of four symbols then last two symbols of extension should form hexadecimal representation of the number N; in this representation the letters 'z', 'a', 'b',..., 'o' carry out a role of the digits having values accordingly 0, 1, 2... 15.

A text file or RTF–file containing a note (see 6.3.3) may correspond to each data file.

6.3.2. Working Language

The working language of the package is the language in which all text messages will be displayed. A list of languages is determined by the existence of files-dictionaries, serving for translation of the messages from English, in the main directory. The user can add new or to remove the existing files-dictionaries (their total number should not exceed 16).

For translation of text messages by the program, in the main directory, there should be a file with the name coinciding with the name of chosen language (Russian, Georgian etc.) and having the extension **.dic** (for example **georgian.dic**), containing a dictionary of translated lines, and also a file with the same name and with extension **.add** (for example **georgian.add**). For representation of the help information in the chosen language, in the main

directory there should also be a file with the same name and with extension **.hlp** (for example **georgian.hlp**) or a file with the same name and with extension **.pdf** (for example **georgian.pdf**), containing this information.

The working language can be chosen from the list on the **ToolBar** or by means of the option of the main menu **Language** (see Figure 6.2). In the first case, accessible languages are those for which there are both files – with extensions **.dic** and **.add**. In the second case, the presence only of the file with extension **.dic** is enough; thus the auxiliary file with extension **.add** is created by pressing the button **Create**.

The file-dictionary with extension **.dic** can be created or changed as it is described in 6.3.1 and is given in **Help** of the package. At each change in this file, it is also necessary to create the corresponding file with extension **.add** in the way described above.

6.3.3. Help Service and Notes

In the software help information of following types are used:

- *help in a status line*: in the moment of moving of the cursor of a mouse above some visual components (sections of menu, buttons, editing windows, etc.) a short information about these components appears in the **Status Bar** and in emerging label;
- *display text from help files*: it is carried out by means of commands of traditional section of menu **Help**;
- *call of the context-dependent information*: in the software as well as in all **Windows**-programs pressing of the key **F1** causes information for that mode in which is the program in that moment.

The general form of the initial format **Help** is shown in Figure 6.9.

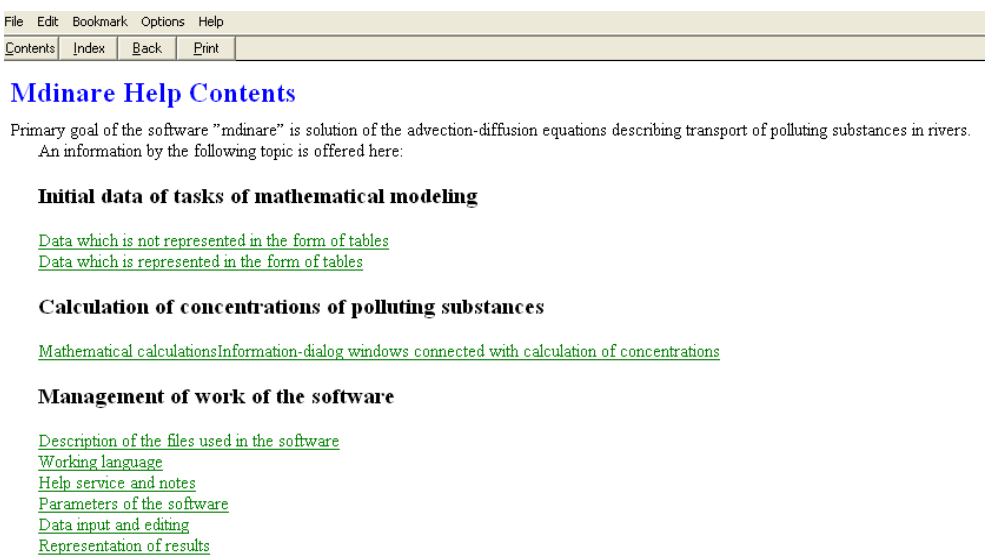


Figure 6.9.

The reference to "help" is not recommended during performance of the program i.e. when calculations are being done in the program.

In all tasks in which initial data are read out from files or any data files are created (in particular they are tasks of data input in tables) the possibility of viewing and editing of notes that is any text corresponding to the used data file or, if there are several such files, to first of them is realized. The file containing a note has the same name and the same directory as corresponding data file and one of the following extensions – **.tex**, **.txt**, **.rtf** depending on its type.

Call of the editor of notes is carried out by the command **Help|Notes**. During editing of the file containing a note its type can be changed.

6.3.4. Parameters of the Package

The change in the value of each parameter is carried out with the help of standard **Windows** components which allow editing the text, choosing the line from the list, setting the indicator etc.

At working with each form containing the main menu, the assignment of parameters is carried out with the help of commands of the main menu from the groups **File**, **Tools** and **Parameters**. Most important parameters could also be determined with the help of the components located on the **ToolBar**.

It is possible to split the parameters used in the package into several groups, which are considered below.

The main parameters of the package which are not used in calculations:

- *Sizes of pages for printing out*; they are changed with the help of the option **File|Page setup** (see Figure 6.10);
- *Working language* (see Item 6.3.2);
- *Working directory* is the directory where data files are looked up at choosing them; it changes at each change of a folder in standard dialogue windows for opening and saving the files.

These parameters are read from the files **mdinare.num** and **mdinare.str** at running of the package (see Item 6.3.1). The option of the menu **Save options** records the values of parameters changed during the operation of the package in this file. The item of the menu **Autosave** contains the indicator which, in the switched-on state, provides the record of changed values of parameters in the files **mdinare.num** and **mdinare.str** at exiting the package.

The parameters of the package which are used in calculations and are not represented as tables: they are the parameters listed in paragraph 6.2. The parameters which are not marked by the sign 'n' in this list, as well as some parameters of the previous group, are read from the file **mdinare.num** and can be saved in this file.

The type of the model, the type of the algorithm, the number of sections of the river and the number of polluting substances are changed by means of the option of the menu **Tools|Model** in the main form of the program.

The type of coordinates is changed by means of the option of the menu **Coordinates|Type of coordinates** in the main form of the program.

The number of polluting sources in each section is changed at editing the tables "**List of objects**".

The parameters determining the accuracy of calculations are changed by means of the option of the menu **Parameters|Accuracy** in the form of the task **"Calculations"**; the parameter n also is changed by means of the option of the menu **Run|Accuracy** in the main form of the program.

Other parameters are changed by means of the option of the menu **Parameters|Task parameters** and **Parameters|Additional parameters** in the form of the task "**Calculations**", and also in the dialogue windows which appear on the screen before running of this task.

The parameters of the package which are used in calculations and are represented as tables: they are sequences of the same elements, which are entered in tables and are saved in separate files (see Item 6.3.5). The data of the considered type which have been saved in files are used in calculations. The concrete tables of initial data used in the package are described in paragraph 6.2.

The parameters of setting of the printer are parameters of **Windows**, which, in particular, are used by the package; they are changed by means of the option **File|Printer setup** (see Figure 6.10).

The parameters determining the type of the diagram at representation of computation results (see paragraph 6.4).

6.3.5. Data Input and Editing

The entered data which form sequences of elements of the same type are represented in the form of tables. When there are several editing windows with tables on the screen, different windows correspond to different sections of the river.

There are the possibilities of entering the data which have not been recorded anywhere, reading data from files and saving them in files by means of commands **File|New**, **File|Open**, **File|Save**, **File|Save as**, **File|Save all** standard for the text and graphic **Windows** editors (see Figure 6.11).

The option **File|Send** records the data in a text file. The option **File|Print** performs printing of the table.

The data files have quite a simple structure (see 6.3.1) and can be created outside of this package.

The data of the package presented in the form of a table can be entered and edited by means of a mouse and a keyboard. There are the possibilities changing, deleting or adding the symbols into the record of the element; deleting or adding new elements in the necessary place; selecting a block of data; moving or copying the selected block to a new place; removing, writing down in a file or reading the block of the data from the file; printing out both the selected block and all contents of the data file.

There are two operating modes with a table of data – the mode of editing of cells and the operating mode with blocks. In the first mode, it is possible to edit the text in each cell of the table, but it is impossible to select a block from several cells. In the second mode, on the contrary, it is possible to select the block from several cells (for copying, removal, insertion etc.), but it is impossible to edit the text.

The switching between these modes is carried out by the button **Edit** on the **ToolBar**.

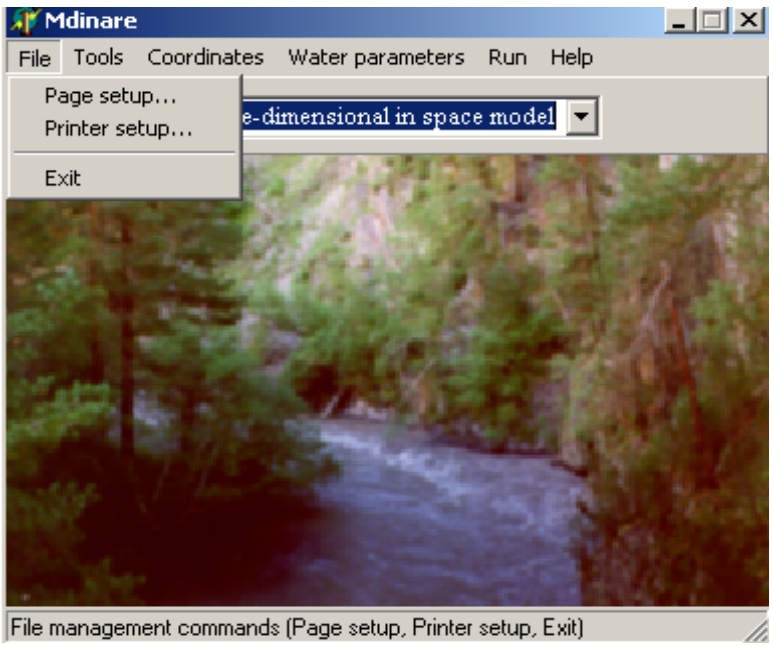


Figure 6.10.

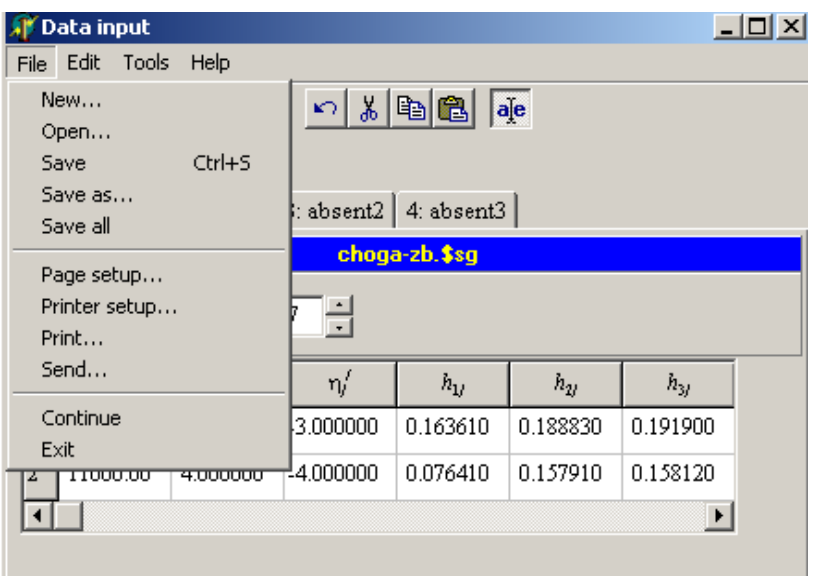


Figure 6.11.

6.4. Realization of Computation and Representation of the Results

The package uses curvilinear coordinates of the points of the river banks and polluting sources at solving the diffusion equations. Therefore, if the user has chosen Cartesian coordinates for data input, all these Cartesian coordinates should be transformed into curvilinear ones. Such transformation is carried out by the command of the main menu of the main form **Convert files** (see Figure 6.3).

The algorithms and analytical methods are used at solving the diffusion equation. They are described in Chapters 1 and 2. For realization of two-dimensional and three-dimensional models, one of the two algorithms may be used depending on user's choice:

1) The classical algorithm in which the difference equation for layers is equivalent to a system of N linear equations for N values of unknown function at nodal points; this system is solved by the iteration method;

2) The algorithm in which the solution of two-dimensional or three-dimensional diffusion equation is represented in the form of a linear combination of solutions of some one-dimensional diffusion equations.

As the experience shows, the second algorithm can be realized by computer much more quickly then the first one.

The method of calculations is also determined by some other parameters listed in paragraph 6.2.

The results of calculations are displayed in the form of text messages, tables, graphs, etc. For example, the formats of display of computation results as diagrams and tables are shown in Figure 6.12 and 6.13, respectively.

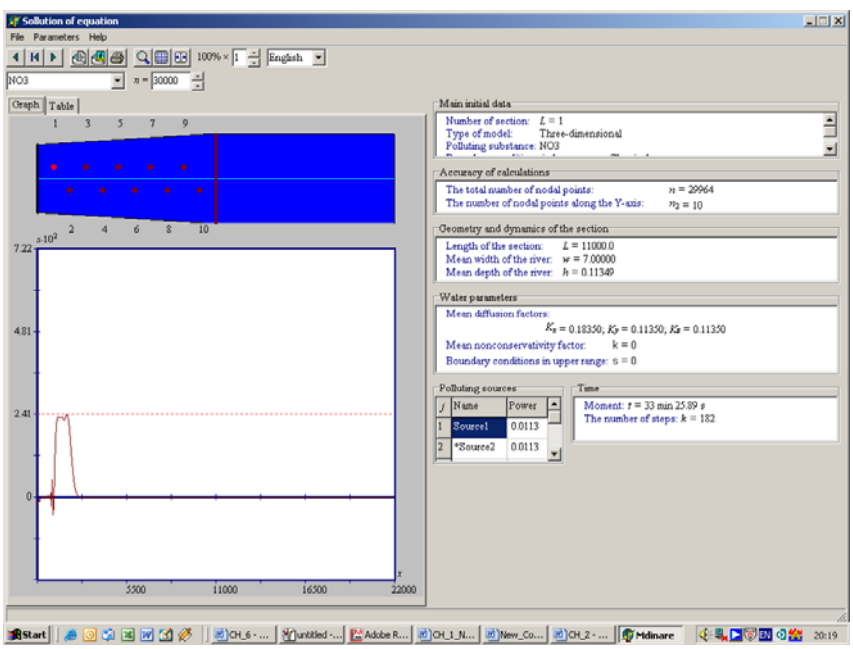


Figure 6.12.

The option **Print** carries out printing of the text and/or the diagram.

The option **Send text** carries out writing of the text in the file name of which is determined by default or indicated by the user. The user can choose one of the following types of files: file **LaTeX** (**tex**-file), a simple text file, text file **MS DOS**. If the saved file already exists on the disk, the user can also set the way of writing of the text by means of the indicator "**Preserve existing text**": to add a new text to the available one or to remove the available text from the file.

It is also possible to single out the text represented on the screen and, by means of combinations of keys **Ctrl-C**, **Ctrl-V**, to move it to the edited document **Word** or to the document of any other editor allowing to work with the text in the **RTF** format.

The option **Send graph** carries out writing of the diagram into the file the name of which is determined by default or indicated by the user. The user can choose one of the following types of files: Metafile (**wmf**-file), Enhanced Metafile (**emf**-file), **Windows Bitmap** (**bmp**-file) or **JPEG** (**jpg**-file). The user can also set the type of figure which will be drawn in a file – black-and-white or coloured, by means of the indicator.

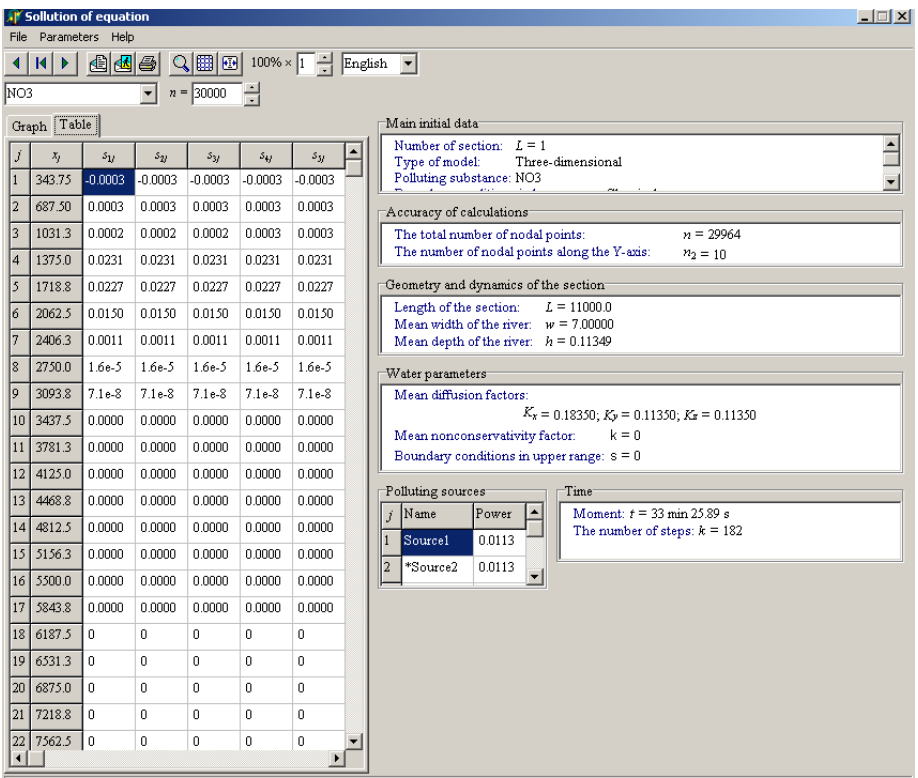


Figure 6.13.

The listed options are called from the main menu or by means of fast buttons of the **ToolBar**, duplicating the corresponding items of the main menu.

The results of calculations together with some initial data are split into groups, which are represented on the screen in various windows. By calling the options **Print** and **Send text,** the

user can select which of the existing groups of data he wants to print or to write down in a file.

In the task "**Calculations**", it is possible to choose the mode of representation of the graph or the table: to represent the graph with a coordinate grid or without it, to increase or to decrease the thickness of lines of a graph, to increase or to decrease the scale of data presentation in the graph, to set the standard or maximum size of the window containing the graph and the table. The parameters determining the view of the screen are changed by means of the command of the menu **Parameters|Graph view** or by means of some components on the **ToolBar**.

See also 6.3.4, 6.3.2, 6.3.3.

Chapter 7

SOFTWARE OF IDENTIFICATION OF THE SOURCES OF EXCESSIVE RIVER POLLUTION

7.1. APPOINTMENT OF THE PACKAGE

The package of applied programs of identification of emergency pollution sources of surface or sewage water created by authors is described in the offered chapter. Despite the urgency the considered problem, as far as we know, is solved by authors of the present work for the first time. They possess publications in which the given problem is theoretically proved and solved [1, 182, 187, 188, 210, 221]. The urgency of the given problem is noted in publications [192-197]. For detection of initiators of emergency pollution of sewage of Odessa nitrogen factory among possible five shops, the simple algorithms based on a method of the cluster analysis and using the elementary model, considering only transfer and dilution of polluting substances in sewage (see paragraph 5.2), have been developed and introduced in the automated monitoring system of sewage of factory under the guidance of author of the given work.

The developed package is intended for automatic identification of sources of emergency dumping in the rivers between two controllable ranges. It is realized for IBM- compatible personal computers in operational systems MS DOS and WINDOWS. The description only WINDOWS-version is given below.

Presence of such package is rather actual for solving the problem of objective control and acceptance of optimum decisions for the purpose of management of processes of formation of quality of river water and water use. For demonstration of its urgency it is enough to notice that work on creation of the given package is executed within the project G-047 ISTC (International Science and Technology Center), based by USA, Japan and the countries of EU. The basic result of the work is the solution of principle of most important task of the problem of monitoring of river water and working out of original working algorithms and the unified computer software for certain set of types of water objects and pollution processes.

The technique realized in the package, methods of the solution of problems, algorithms and programs of their realization are original, belong to authors and have not analogues. In particular, the algorithms of identification based on methods of the cluster-analysis and the theory of acceptance decisions, used depending on the volume of the available a priori information, by increasing of which it is possible to apply more complex procedures of

acceptance decisions, providing higher reliability, are developed. For latest case, i.e. in the presence of the sufficient a priori information, there are developed optimum (iterative) and quasi-optimum (analytical) algorithms of identification of emergency pollution sources of river water (see Chapter 4). Mathematical models of transferring polluting substances in the rivers taking into account their features and specificity of sources and pollution processes are created. In particular, one-, two- and three-dimensional diffusion models of transferring pollutants at different initial and boundary conditions depending on specificity of formation of quality of water stream (see Chapters 1, 2, 3). The quantitative estimations are obtained, allowing to define borders of action of the developed models depending on features of the water stream, the characteristic of polluting substances and the form of their dump (see Chapter 8).

7.2. POSSIBILITY OF THE PACKAGE AND ITS APPLICATION

The necessary initial information characterizing geographical and hydrological features of the considered section of water object, form and pollution process of this section from natural and artificial pollution sources is introduced in the package; methods of solution on the basis of afore-named features of water object and final goals for which achievement the given problem is considered are chosen and at occurrence of a situation of emergency pollution, by starting of the given package, the set of the most probable sources of this not authorized pollution is automatically found out.

The input information for the developed package are: quantity of pollution sources and their spatial co-ordinates, spatial co-ordinates and the list of measured parameters on which the river control is carried out, the name and concentration of dumped substances by pollution sources in normal and possible emergency operation of functioning, the characteristic of features of the river and conditions of descent of sewage. Besides the aforesaid, service functions of input-output, editing, graphic representation of output data are realized in the package. There is a standard access to each program of the package (the detailed description is given in the instruction of the user in Help). All these functions are realized in the given package similarly to corresponding functions of the package of mathematical models of transportation of pollutants in the rivers, described in Chapter 6. Therefore here it is not resulted their detailed description. The names of the options realized in the package for introduction of input information and calculations are shown on Figure 7.1. They basically are similar to corresponding options of the previous package, except the options “Prelim. calculations” and “Decision making” of the section “Run” of the basic menu. The form of the format of the option “Decision making” is shown on Figure 7.2. The choice of a method of making the decision from described in Chapter 4 and in paragraph 5.7 is carried out in this mode.

The graphic form of output information of the package on which on the scheme of the considered section of the river by red points are specified pollution sources of the given section by considered parameter is resulted on Figure 7.3. Among all pollution sources brightly red colour allocates the sources, guilty of emergency pollution. The list of all pollution sources with indication of the made decision about its guilt is given in the bottom right corner: **Non guilty** (it is not guilty), **Guilty** (it is guilty) and **Controlled** (supervised).

Along to each object two figures are specified: the first – number of the considered section of the river, the second – the serial number of object of pollution within the considered section. **It is not guilty** means that the given pollution source is not emergency polluter in the considered situation, **it is guilty** means that the given pollution source is emergency polluter in the considered situation and **controllable** means that sewage of the given source of pollution are supervised directly ahead of dump in considered water object and there is not any uncertainty concerning its role in the process of pollution. The table of the generated hypotheses concerning guilt in emergency pollution of sources of dumps with indication of corresponding concentrations of the considered component of pollution is given in the bottom left corner.

Capacity of work of the software was tested in the diverse modes of operation; the received results confirm stability and reliability of algorithms and also high accuracy of computed values (see Chapter 8 (paragraph 8.2)).

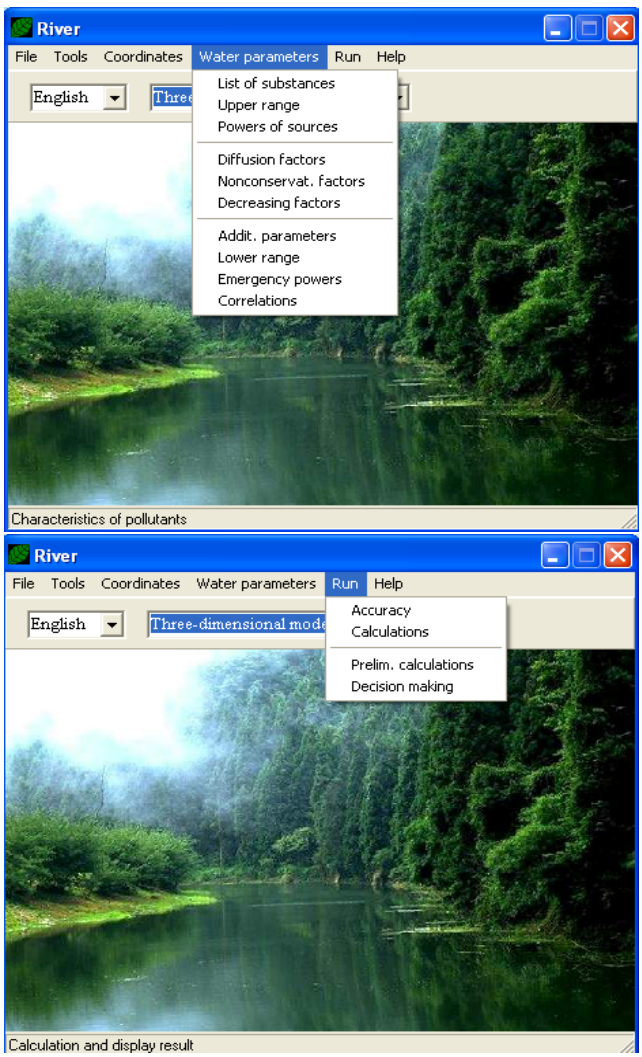


Figure 7.1. The modes of operation of input information and computations realized in the package.

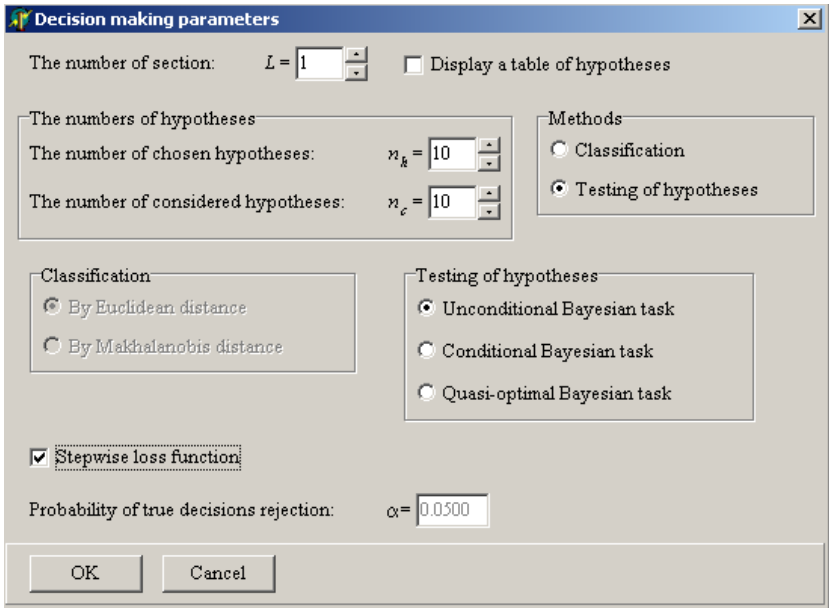


Figure 7.2.

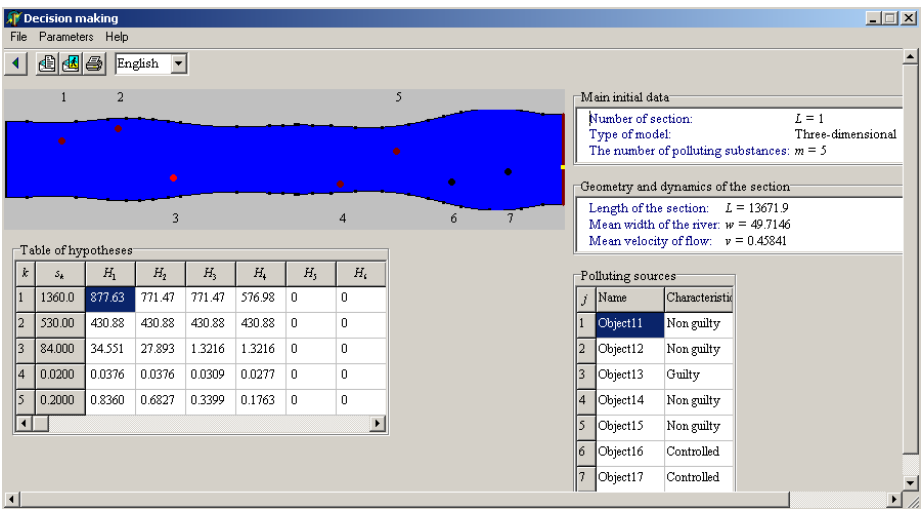


Figure 7.3. Graphic view of output information of the package.

There is the possibility of the choice of a language of dialogue with the package from the set of the languages realized in it. Besides for WINDOWS version, the user can, without special efforts, independently to add any, him interesting language to languages of dialogue with the package. For this purpose extremely simple instruction is given in Help. Concerning these possibilities see description of the previous package in Chapter 6.

It is necessary to underline especially that the offered package (as well as previous) is completely original as all algorithms, programs, texts, graphs, drawings, tables, designs etc. realized in this package, are original, belong to authors, and have not analogues.

Chapter 8

INVESTIGATION OF DEVELOPED ALGORITHMS AND PROGRAMS

The results of experimental research, developed in Chapters 1 and 2 algorithms and appropriate programs, included in computer packages and described in Chapters 6 and 7, are given below. The results of research of algorithms of calculation of concentration of polluting substances in the rivers with the help of diffusion equations and also sensitivity of models of different dimensions to the geometrical sizes of a section of the river and dependence of quality of identification of emergency pollution sources on the level of the noise, deforming results of measurement, are considered. The results of calculation of distribution of concentration of polluting substances in some rivers of the Western Georgia are reduced. By means of computer modelling mid-annual quantities of some polluting substances which have got on certain sections of the rivers of r. Khobistskali's (Western Georgia) basin, between control sections from sources of pollution operating on these sections, and the mid-annual quantity of these substances brought by them to Black sea are calculated.

The results of research of algorithms of making decisions, developed in Chapter 4, are brought in the end of the same chapter in paragraph 4.6. They show truth and reliability both the created algorithms and programs of their realization. The results of research of dependence of quality of algorithms of identification of emergency pollution sources from the level of the noise, imposed on the results of measurement, are reduced in the present chapter.

8.1. STUDY OF ALGORITHMS FOR CALCULATION OF POLLUTANT CONCENTRATIONS IN RIVERS BY MEANS OF DIFFUSION EQUATIONS

The program system for numerical realization of the problems of pollutants transport in water flows consist of three main parts: 1) the programs realizing one-dimensional problems; 2) the programs realizing two-dimensional problems; 3) the programs realizing three-dimensional problems.

The programs were mainly developed on the base of finite-difference algorithms described in Chapter 2. For some problems of a specific character, the analytical method was used.

The main program modules used in all the parts are: 1) the program realizing the run method – the factorization method; 2) the program for solution of two- and three- dimensional implicit finite difference equation; this program is based on the Gaussian-Zeidel iterative method.

Testing of the program system was carried out for specially selected test problems. Numerical experiments were carried out in order to detect mechanical errors made during algorithmic presentation or programming; to test the robustness against the initial data, the accuracy of the results obtained, and the calculation time; to compare different algorithms, etc.

Particular attention was given to carrying-out of computational experiments in the case of pollution sources of a special type (an instantaneous point or stretched source), oscillations in solutions of equations at peculiarities in the initial data, etc.

The numerical experiments gave the following results:

1) In the case of classical one-dimensional problems, certain computational capabilities were shown by the purely implicit scheme and the Crank-Nicolson scheme; in the case of special loads, it is preferable to use the purely implicit scheme, but in the case of smooth initial data – the Crank-Nicolson scheme.
2) In the case of non-classical boundary conditions (non-local conditions), the used finite difference algorithms showed the same capabilities as in the classical case.
3) In the two-dimensional case, the experiments were carried out on the base of the parallel calculating decomposition schemes and the two-dimensional implicit scheme as well as the two-dimensional Crank-Nicolson scheme; in terms of the calculation time, the decomposition scheme is more preferable; it should be noted that the paralleling feature of decomposition schemes was not used in the calculation; in terms of the accuracy, in the case of smooth initial data, the best capabilities were shown by the Crank-Nicolson algorithm with the use of the Gaussian-Zeidel iterative process, which quite agrees with the theoretical studies.
4) In the case of non-classical two-dimensional problems, the experiments were only carried out by means of the decomposition schemes; in this case, all the theoretical predictions concerning the used algorithms were confirmed.
5) When compared with each other, the used three-dimensional algorithms showed the same features and capabilities as the corresponding two-dimensional algorithms. Certainly the increase in the dimensionality of the problem affected the possibility of increasing the accuracy of calculations; the same holds true for the case of non-classical (non-local) initial-boundary problems.

To verify the above mentioned in Appendix 5 are given the graphs of realization of some specially selected tests. These tests are based on the exact solutions of the corresponding one-, two- and three- dimensional equations. By their character, the tests represent two types of solution classes: smooth non-oscillating functions and oscillating functions. Comparison of the presented graphs shows the influence of these features on the accuracy of calculations.

It should be noted that the exact solutions are shown on the graphs by points, while the approximate solutions – by full curves. For multidimensional cases, the graphs for different z and y are given in one and the same figure. For calculation, were used the tests described below.

Designations

T – the time of calculation;
L – the number of layers;
$t = L \cdot \tau$ - the current time;
n_x, n_y, n_z - the numbers of steps along axes x, y, z;
N – the total number of points;
$\max\left\{\Delta\Phi_j\right\}$ - maximum absolute deviation;
$\max\left\{\Delta\Phi_j / \Phi_j\right\}$ – the maximum relative deviation.

Bounds

$-1 \le x \le 5$; $-0.5 \le y \le 3.5$; $-0.3 \le z \le 2.7$.

One-dimensional Model. Function I

Considered Function

$$\Phi_1^{ex}(A, B, \lambda, \mu; x) \equiv A \cdot e^{\lambda x} + B \cdot e^{\mu x},$$

Considered Equation

$$D \cdot \partial_t \Phi(x,t) - \partial_x^2 \Phi(x,t) + (\lambda + \mu) \cdot \partial_x \Phi(x,t) + (k^2 - \lambda\mu) \cdot \Phi(x,t) = f(x) \cdot \exp(-tk^2 / D),$$

Function

$$\Phi(x,t) = \Phi_1^{ex}(A, B, \lambda, \mu; x) \cdot \exp(-tk^2 / D),$$

where A, B, λ, μ - the selected model parameters (arbitrary constants), is the solution of the equation at $f(x) = 0$.

Function

$$\Phi(x,t) = \Phi_1^{ex}(A,B,\lambda,\mu;x)\cdot e^{-t\kappa^2/D} + \Phi_1^{ex}(\widetilde{A},\widetilde{B},\widetilde{\lambda},\widetilde{\mu};x)\cdot e^{-t\kappa^2/D},$$

where $\widetilde{A},\widetilde{B},\widetilde{\lambda},\widetilde{\mu}$ - the additional selected model parameters (arbitrary constants), is the solution of the non-homogeneous equation at

$$f(x) = -\widetilde{A}\cdot(\widetilde{\lambda}-\lambda)\cdot(\widetilde{\lambda}-\mu)\cdot e^{\widetilde{\lambda}x} - \widetilde{B}\cdot(\widetilde{\mu}-\lambda)\cdot(\widetilde{\mu}-\mu)\cdot e^{\widetilde{\mu}x}.$$

One-dimensional Model. Function II

Considered Function

$$\Phi_1^{si}(A,B,\omega,s;x) \equiv e^{sx}\cdot(A\cdot\cos(\omega x) + B\cdot\sin(\omega x)).$$

Considered Equation

$$D\cdot\partial_t\Phi(x,t) - \partial_x^2\Phi(x,t) + 2s\cdot\partial_x\Phi(x,t) + (k^2-\omega^2-s^2)\cdot\Phi(x,t) = f(x)\cdot\exp(-tk^2/D).$$

Function

$$\Phi(x,t) = \Phi_1^{si}(A,B,\omega,s;x)\cdot\exp(-tk^2/D),$$

where A,B,ω,s – the selected model parameters (arbitrary constants), is the solution of the equation at $f(x)=0$.

Function

$$\Phi(x,t) = \Phi_1^{si}(A,B,\omega,s;x)\cdot e^{-t\kappa^2/D} + \Phi_1^{si}(\widetilde{A},\widetilde{B},\widetilde{\omega},\widetilde{s};x)\cdot e^{-t\kappa^2/D},$$

where $\widetilde{A},\widetilde{B},\widetilde{\omega},\widetilde{s}$ - the additional selected model parameters (arbitrary constants), is the solution of the non-homogeneous equation at

$$f(x) = \widetilde{A}\cdot\left(\left(\widetilde{\omega}^2-\omega^2-(\widetilde{s}-s)^2\right)\cdot W_1 + 2\widetilde{\omega}\cdot(\widetilde{s}-s)\cdot W_2\right) + \\ + \widetilde{B}\cdot\left(\left(\widetilde{\omega}^2-\omega^2-(\widetilde{s}-s)^2\right)\cdot W_2 + 2\widetilde{\omega}\cdot(s-\widetilde{s})\cdot W_1\right),$$

where

$$W_1 = e^{\widetilde{s}x}\cdot\cos(\widetilde{\omega}x); \quad W_2 = e^{\widetilde{s}x}\cdot\sin(\widetilde{\omega}x).$$

Two-dimensional model. Function I

Considered Equation

$$D\cdot\partial_t\Phi(x,y,t)-\partial_x^2\Phi(x,y,t)-\partial_y^2\Phi(x,y,t)+(\lambda_1+\mu_1)\cdot\partial_x\Phi(x,y,t)+$$
$$+(\lambda_2+\mu_2)\cdot\partial_y\Phi(x,y,t)+(k^2-\lambda_1\mu_1-\lambda_2\mu_2)\cdot\Phi(x,y,t)=f(x,y)\cdot\exp(-tk^2/D),$$

Function

$$\Phi(x,y,t)=\Phi_1^{ex}(A_1,B_1,\lambda_1,\mu_1;x)\cdot\Phi_1^{ex}(A_2,B_2,\lambda_2,\mu_2;y)\cdot\exp(-tk^2/D),$$

where $A_1,B_1,\lambda_1,\mu_1,A_2,B_2,\lambda_2,\mu_2$ – the selected model parameters (arbitrary constants), is the solution of the equation at $f(x,y)=0$.

Function

$$\Phi(x,y,t)=\Phi_1^{ex}(A_1,B_1,\lambda_1,\mu_1;x)\cdot\Phi_1^{ex}(A_2,B_2,\lambda_2,\mu_2;y)\cdot e^{-t\kappa^2/D}+$$
$$+\Phi_1^{ex}(\widetilde{A}_1,\widetilde{B}_1,\widetilde{\lambda}_1,\widetilde{\mu}_1;x)\cdot\Phi_1^{ex}(\widetilde{A}_2,\widetilde{B}_2,\widetilde{\lambda}_2,\widetilde{\mu}_2;y)\cdot e^{-t\kappa^2/D},$$

where $\widetilde{A}_1,\widetilde{B}_1,\widetilde{\lambda}_1,\widetilde{\mu}_1,\widetilde{A}_2,\widetilde{B}_2,\widetilde{\lambda}_2,\widetilde{\mu}_2$ - selected model parameters (arbitrary constants), is the solution of the non-homogeneous equation at

$$f(x,y)=f_1(x)\cdot\Phi_1^{ex}(\widetilde{A}_2,\widetilde{B}_2,\widetilde{\lambda}_2,\widetilde{\mu}_2;y)+f_2(y)\cdot\Phi_1^{ex}(\widetilde{A}_1,\widetilde{B}_1,\widetilde{\lambda}_1,\widetilde{\mu}_1;x),$$

where

$$f_1(x)=-\widetilde{A}_1\cdot(\widetilde{\lambda}_1-\lambda_1)\cdot(\widetilde{\lambda}_1-\mu_1)\cdot e^{\widetilde{\lambda}_1 x}-\widetilde{B}_1\cdot(\widetilde{\mu}_1-\lambda_1)\cdot(\widetilde{\mu}_1-\mu_1)\cdot e^{\widetilde{\mu}_1 x};$$
$$f_2(x)=-\widetilde{A}_2\cdot(\widetilde{\lambda}_2-\lambda_2)\cdot(\widetilde{\lambda}_2-\mu_2)\cdot e^{\widetilde{\lambda}_2 x}-\widetilde{B}_2\cdot(\widetilde{\mu}_2-\lambda_2)\cdot(\widetilde{\mu}_2-\mu_2)\cdot e^{\widetilde{\mu}_2 x}.$$

Two-dimensional Model. Function II

Considered Equation

$$D\cdot\partial_t\Phi(x,y,t)-\partial_x^2\Phi(x,y,t)-\partial_y^2\Phi(x,y,t)+2s_1\cdot\partial_x\Phi(x,y,t)+2s_2\cdot\partial_y\Phi(x,y,t)+$$
$$+(k^2-\omega_1^2-s_1^2-\omega_2^2-s_2^2)\cdot\Phi(x,y,t)=f(x,y)\cdot\exp(-tk^2/D).$$

Function

$$\Phi(x,y,t)=\Phi_1^{si}(A_1,B_1,\omega_1,s_1;x)\cdot\Phi_1^{si}(A_2,B_2,\omega_2,s_2;y)\cdot\exp(-tk^2/D),$$

where $A_1,B_1,\omega_1,s_1,A_2,B_2,\omega_2,s_2$ – the selected model parameters (arbitrary constants), is the solution of the equation at $f(x,y)=0$.

Function

$$\Phi(x,y,t)=\Phi_1^{si}(A_1,B_1,\omega_1,s_1;x)\cdot\Phi_1^{si}(A_2,B_2,\omega_2,s_2;x)\cdot e^{-t\kappa^2/D}+$$
$$+\Phi_1^{si}(\widetilde{A}_1,\widetilde{B}_1,\widetilde{\omega}_1,\widetilde{s}_1;x)\cdot\Phi_1^{si}(\widetilde{A}_2,\widetilde{B}_2,\widetilde{\omega}_2,\widetilde{s}_2;x)\cdot e^{-t\kappa^2/D},$$

where $\widetilde{A}_1,\widetilde{B}_1,\widetilde{\omega}_1,\widetilde{s}_1,\widetilde{A}_2,\widetilde{B}_2,\widetilde{\omega}_2,\widetilde{s}_2$ - the additional selected model parameters (arbitrary constants), is the solution of the non-homogeneous equation at

$$f(x,y)=f_1(x)\cdot\Phi_1^{si}(\widetilde{A}_2,\widetilde{B}_2,\widetilde{\omega}_2,\widetilde{s}_2;y)+f_2(y)\cdot\Phi_1^{si}(\widetilde{A}_1,\widetilde{B}_1,\widetilde{\omega}_1,\widetilde{s}_1;x),$$

where

$$f_1(x)=\left(-\partial_x^2+2s_1\cdot\partial_x+(\kappa^2-s_1^2-\omega_1^2)\right)\Phi_1^{si}(\widetilde{A}_1,\widetilde{B}_1,\widetilde{\omega}_1,\widetilde{s}_1;x);$$
$$f_2(x)=\left(-\partial_x^2+2s_2\cdot\partial_x+(\kappa^2-s_2^2-\omega_2^2)\right)\Phi_1^{si}(\widetilde{A}_2,\widetilde{B}_2,\widetilde{\omega}_2,\widetilde{s}_2;x).$$

Three-Dimensional Model

In the case of the three-dimensional model, the equations similar to those of the two-dimensional model are considered. The solutions of these equations are formed by functions Φ_1^{ex} and Φ_1^{si} in analogous to the two-dimensional model way.

8.2. Complex Testing of the Developed Package

8.2.1. Sensitivity of the Models of Different Dimensionality to Geometric Sizes of the River Cross-Section

It is known from the hydrology of rivers that, if one of the geometric sizes of the considered river section exceeds the other more than ten times, the latter may be neglected in computations as it does not affect the calculation results [5]. For checking this fact by means of the developed models, we calculated the transport of pollutant concentrations for different geometric sizes of the considered river section. There are seven pollution sources located

along the river section. The discharge points of these sources are located uniformly on the diagonal of the river section. The resultant concentration was calculated for the middle point of the lower cross-section of the controlled river section for different pollution sources separately. The diffusion coefficients are $K_x = K_y = K_z = 0.2$, non-conservative coefficient is $K = 0$. The cross-section area and the average river flow velocity in the lower cross-section were changed in accordance with the river width and depth at equal flow rates.

At the river geometric sizes: length – 1000 m, width – 90 m, depth – 3 m, the one-, two- and three-dimensional models gave absolutely similar results.

At the river geometric sizes: length – 1000 m, width – 150 m, depth – 3 m, two- and three-dimensional models gave similar results, different from those of the one-dimensional model.

At the river geometric sizes: length – 1000 m, width – 150 m, depth – 50 m, all the three models gave different results.

From these calculations, the following practical recommendation concerning the use of the developed models may be given. If geometric sizes, locations of pollution sources, hydrologic characteristics and pollution conditions of the river are such that full mixing of water takes place upstream of the lower controlled section, then it is enough to use the one-dimensional river models, which are considerably faster and require less computer memory than the models of greater dimensionality. Otherwise it is necessary to use the models of greater dimensionality.

When choosing a working model for a concrete section of a certain river, it is necessary to perform preliminary studies with due regard for the above factors. The proper choice of the model and its parameters ensures the qualitative modeling and identification of excessive discharge sources.

8.2.2. Dependence of the Identification Quality on the Noise Level

To illustrate the proper functioning of the developed program package for identification of river water pollution sources (see Chapter 7), let's consider the following example [210].

There are five uncontrolled and two controlled pollution sources between the $(j-1)$-th and the j-th controlled sections. River water quality indices in these ranges, noise variance $\overline{X}_0^{(j)}(t)$ and discharged concentrations in normal y_{ir} and excessive $y_{ir\max}$ modes are given in Table 8.1. It is taken: $E(\overline{x}_{i0}^{j}(t)) = 0,\ V(\overline{x}_{i0}^{j}(t)) = \sigma_{io}^2;\ \mu_{ij}$ - the maximum allowable concentration (MAC) of the i-th ingredient in the j-th section. The concentrations of chlorides, sulphates and ammonia nitrogen exceed the corresponding MACs, which shows that the pollution exists in the j-th section. The following characteristics of the river and pollution processes are taken: length, width and depth of the river – 1000 m, 50 m, and 3 m, respectively, i.e. the river within the considered section is one-dimensional by its nature. Therefore, the identification is carried out by means of the one-dimensional models. The diffusion and non-conservativity coefficients for pollutants are $K_x = 0.2$ and $K = 0$, respectively. The cross-section area and average river flow velocity in the lower cross-section

are 150 m^2 and 1/3 m/s, respectively. The pollution sources are located along the considered river section at equal intervals, i.e. the interval between them is ~125 m. The duration of discharge from each source is an hour.

For the lower cross-section measurement vector given in Table 8.1, hypothetical combinations of excessive pollution sources given in Table 8.2 were chosen. Of course, the change in the measurement vector involved the change in the hypothetical combinations of excessive pollution sources.

Table 8.3 gives the identification results obtained by means of different algorithms of making decision at generation of five measurement results with identical variances according to the following formula $x_{imes} = x_{i,j} + k \cdot N(x|0;\sigma_{i0}),\ k = 0,1,...,4;$ where $N(x|0;\sigma_{i0})$ – the normally distributed random variable with mathematical expectation equal to zero and variance σ_{i0}^2. For testing of the conditional and un conditional algorithms of testing hypotheses when the number of hypotheses is equal to two, the number of hypotheses was artificially reduced to two by choosing those two hypotheses that are the closest to the measurement point. The results of computations show that, at noise variances given in Table 8.1, all the algorithms give true decisions (the H_1 hypothesis in the considered case) in 100% of the cases. As the noise variance increases, the number of falsely made decisions increases. The conditional Bayesian algorithm of many-hypotheses testing works best of all, next is the unconditional Bayesian algorithm.

The power of the hypotheses testing rule in the conditional and quasi-optimal Bayesian algorithms is $1-\alpha = 0.95$. As the noise variances increased, the mean risk values calculated in the Bayesian problems of many-hypotheses testing, naturally, increased.

The same example was repeated for two- and three-dimensional cases of the river section (see section 8.1). The results of the package operation do not practically differ from those of the one-dimensional case.

Multiple recurrence for different generated groups of normally distributed noise vectors did not change the qualitative relationship in the results of algorithms for identification of the excessive discharge sources. For the considered example, at using the algorithms based on Euclidean, Makhalanobis distances, quasi-optimal, unconditional and conditional Bayesian algorithms when the number of hypotheses is two, the time needed for identification of the sources guilty of the excessive discharges makes up several sec, while at using the unconditional and conditional optimal Bayesian algorithms, it makes up greater than ≈ 3 and ≈ 10 times, respectively.

When choosing hypotheses testing algorithm for a concrete section of a certain river, it is necessary to study the noise level preliminarily, because, at low noise level, simple algorithms requiring minimum calculation time and inconsiderable computer memory can be used.

Table 8.1.

#	Water quality index	Upper range $x_{i,j-1}$	Uncontrolled objects					Controlled objects		σ_{i0}	Lower range $x_{i,j}$	MAC μ_{ij}
			OB1 $\frac{y_{1r}}{y_{1r\max}}$	OB2 $\frac{y_{2r}}{y_{2r\max}}$	OB3 $\frac{y_{3r}}{y_{3r\max}}$	OB4 $\frac{y_{4r}}{y_{4r\max}}$	OB5 $\frac{y_{5r}}{y_{5r\max}}$	OB6	OB7			
1	Flow rate. m^3/s	50	$\frac{1}{5}$	$\frac{0.5}{1.0}$	$\frac{0.7}{1.2}$	$\frac{0.8}{1.4}$	$\frac{0.3}{0.7}$	0.4	0.3	6	59	-
2	Chlorides. mg/l	300	$\frac{400}{10500}$	$\frac{300}{8000}$	$\frac{500}{9000}$	-	$\frac{200}{7000}$	100	90	20	1519	350
3	Sulphates. mg/l	350	$\frac{700}{2300}$	-	$\frac{600}{2100}$	-	-	300	250	10	592	500
4	Ammonia nitrogen. mg/l	1.4	$\frac{5}{800}$	-	-	$\frac{8}{1000}$	$\frac{3}{500}$	1.6	1.5	0.2	81	2.00
5	Petroleum products. mg/l	0.027	-	$\frac{0.04}{0.20}$	$\frac{0.05}{0.25}$	$\frac{0.07}{0.3}$	-	0.03	0.02	0.002	0.03	0.05
6	Iron. mg/l	0.17	-	$\frac{1}{10}$	-	$\frac{2}{15}$	$\frac{1.5}{13}$	0.2	0.15	0.01	0.41	0.50

Table 8.2.

Hypothesis number	Objects (enterprises) suspected in pollution	Values of parameters measured in the lower controlled range				
		Chlorides, mg/l	Sulphates, mg/l	Ammonia nitrogen, mg/l	Petroleum products, mg/l	Iron, mg/l
H_1^*	OB1, OB2	1519.53	592.28	81.56	0.03	0.41
H_2	OB1, OB2, OB4	1519.53	592.28	109.44	0.04	0.80
H_3	OB1, OB3	1616.33	592.28	88.54	0.03	0.59
H_4	OB1, OB2, OB5	1616.33	592.28	116.42	0.04	0.97
H_5	OB1	1362.53	592.28	81.56	0.03	0.22
H_6	OB1, OB2, OB4, OB5	1728.53	634.28	109.44	0.04	0.80

* - show true hypotheses for measurement results from table 8.1
OB1,...,OB5 – the first, the second,…, fifth objects accordingly.

Table 8.3.

#	Method of decision making	**Accepted hypotheses at five different experiments**				
		$x_{imes} = x_{ij}$	$x_{imes} = x_{ij} + N(x/0;\sigma_{i0})$	$x_{imes} = x_{ij} + 2 \cdot N(x/0;\sigma_{i0})$	$x_{imes} = x_{ij} + 3 \cdot N(x/0;\sigma_{i0})$	$x_{imes} = x_{ij} + 4 \cdot N(x/0;\sigma_{i0})$
1.	Euclidean distance	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_2, H_1,$ H_1, H_2	$H_1, H_2, H_3,$ H_3, H_2	$H_1, H_2, H_3,$ H_6, H_2
2.	Makhalanobis distance	H_1	$H_5, H_1, H_5,$ H_1, H_1	$H_1, H_1, H_5,$ H_5, H_1	$H_1, H_2, H_5,$ H_5, H_2	$H_3, H_2, H_5,$ H_5, H_2
3.	Unconstrained at $S = 2$	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_2, H_1,$ H_1, H_2	$H_1, H_2, H_3,$ H_3, H_2
4.	Constrained at $S = 2$	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_2, H_1,$ H_1, H_2	$H_1, H_2, H_3,$ H_3, H_2
5.	Quasi-optimal	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_2, H_1,$ H_1, H_2	$H_1, H_2, H_3,$ H_1, H_2
6.	Unconstrained	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_3,$ H_1, H_1	$H_1, H_1, H_3,$ H_3, H_1
7.	Constrained	H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_1, H_1	$H_1, H_1, H_1,$ H_3, H_1	$H_1, H_1, H_1,$ H_1, H_1

8.3. MODELING OF POLLUTANTS TRANSPORT IN RIVERS

The initial data and computation results for two rivers – the Chogha and the Khobistskali from the basin of the River Khobistskali flowing in Georgia located in the Caucasus are submitted below. The basin of the River Khobistskali is located in Western Georgia and includes four main rivers: the Chogha, the Ochkhomuri, the Chanistskali and the Khobistskali. The main of them is the River Khobistskali, an upstream tributary of which is the Ochkhomuri, and a downstream tributary is the Chanistskali. The Chogha flows into the Ochkhomuri. The Khobistskali is a river of a medium size, about 75 km in length and one meter in mean depth. The River Chogha is a small river: about 12 km in length and 20 centimeters in mean depth. The map of the region of Western Georgia, on which the rivers of the Khobistskali basin and the sections, in where the monitoring in 2002 – 2004 years was executed are marked, is shown in Figure 8.1. On the map, those sections are marked only the observation results of which were used for modeling. As is obvious from the map, the Khobistskali flows into the Black Sea. Simulation of the spread of pollutants in the considered rivers was executed by pollution parameters NO_3 and PO_4. It should be borne in mind that the observation results for the considered rivers can vary considerably within a year.

8.3.1. The Initial Data for Modeling

Spread of pollution in the rivers is modeled for the Chogha between points 1 and 2 and for the Khobistskali between points 3 and 4 (see Figure 8.1).

8.3.1.1. The River Chogha

This river along its full length is fed by unpolluted underground waters. The model in which 10 point sources are evenly distributed lengthwise of the section is considered. Let's cite the data according to which the spread of the above pollutants in the river was modeled.

8.3.1.2. The River Khobistskali

The section of the river between points 3 and 4 (see Figure 8.1) is considered. The pollution sources of the Khobistskali are the Ochkhomuri and the Chanistskali.

Table 8.4. The initial data for the river Chogha: Banks and the bottom; $m = 7$, $N = 2$

j	ξ_j	η_j	$\eta_j^{'}$	h_{1j}	h_{2j}	h_{3j}	h_{4j}
1	0.0	3.0	-3.0	0.16361	0.18883	0.19190	0.14569
2	11 000.0	4.0	-4.0	0.07641	0.15791	0.15812	0.17667

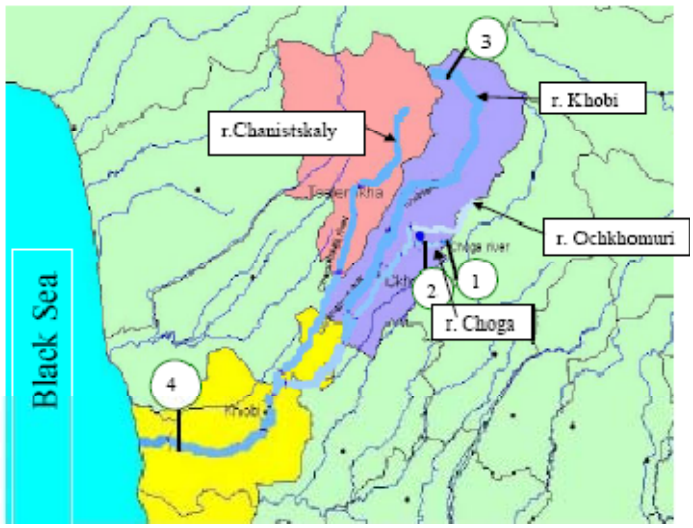


Figure 8.1. The map of region of the western Georgia with the simulated rivers.

Table 8.5. The initial data of flow velocity for the river Chogha: $N = 2$

j	v_j
1	0.535710
2	0.836240

Table 8.6. The initial data of NO_3 and PO_4 in the upper cross-section of the river Chogha: $N = 2$

j	Name	σ_j
1	NO3	3.780000
2	PO4	0.049000

Table 8.7. The initial data of pollution objects of the river Chogha: $N = 10$

j	Name	T_j	ξ_j	η_j	z_j
1	Source1	∞	1000.000	1.000000	0.100000
2	Source2	∞	2000.000	-1.000000	0.100000
3	Source3	∞	3000.000	1.000000	0.100000
4	Source4	∞	4000.000	-1.000000	0.100000
5	Source5	∞	5000.000	1.000000	0.100000
6	Source6	∞	6000.000	-1.000000	0.100000
7	Source7	∞	7000.000	1.000000	0.100000
8	Source8	∞	8000.000	-1.000000	0.100000
9	Source9	∞	9000.000	1.000000	0.100000
10	Source10	∞	10000.000	-1.000000	0.100000

Table 8.8. The initial data of capacities of pollution sources of the river Chogha: $N = 10$

$j \setminus k$	1: Expense	2: NO_3	3: PO_4
1: Source1	0.015000	0.756000	0.009800
2: Source2	0.015000	0.756000	0.009800
3: Source3	0.015000	0.756000	0.009800
4: Source4	0.015000	0.756000	0.009800
5: Source5	0.015000	0.756000	0.009800
6: Source6	0.015000	0.756000	0.009800
7: Source7	0.015000	0.756000	0.009800
8: Source8	0.015000	0.756000	0.009800
9: Source9	0.015000	0.756000	0.009800
10: Source10	0.015000	0.756000	0.009800

Table 8.9. The initial data of diffusion factors in the upper cross-section of the river Chogha: $N = 2$

j	Parameter	K_x	$K_x^{'}$	K_y	$K_y^{'}$	K_z	$K_z^{'}$
1	NO_3	0.181	0.186	0.111	0.116	0.111	0.116
2	PO_4	0.551	0.556	0.521	0.526	0.521	0.526

Table 8.10. The initial data of non-conservativity factors (on the upper) and self-clarification factors (on the lower) in the upper cross-section of the river Chogha: $N = 2$

j	Parameter	l_j	q_j
1	NO3	1000.000	0.991000
2	PO4	1000.000	0.992000

j	Parameter	ζ_j	$\zeta_j^{'}$
1	NO3	0	0
2	PO4	0	0

Table 8.11. Initial data for the river Khobistskali. Banks and the bottom; $m = 7$, $N = 7$

j	ξ_j	η_j	$\eta_j^{'}$	h_{1j}	h_{2j}	h_{3j}	h_{4j}
1	0.0	29.50000	-29.50000	0.404140	0.666970	0.866140	0.593750
2	12000.00	27.75000	-27.75000	0.483765	0.795620	1.127590	0.605275
3	24000.00	26.00000	-26.00000	0.563390	0.924270	1.389040	0.616800
4	28000.00	29.50000	-29.50000	0.562940	0.632900	0.799310	0.804690
5	35500.00	30.00000	-30.00000	1.051675	0.789570	0.801300	0.754485
6	43000.00	30.50000	-30.50000	1.540410	0.946240	0.803290	0.704280
7	44800.00	47.50000	-47.50000	1.540410	0.946240	0.803290	0.704280

Table 8.12. Initial data for flow velocity of the river Khobistskali: $N = 2$

j	v_j
1	0.534930
2	0.796240

Note: In the given Table are given the values of the velocity in two sections of the River Khobistskali – at the beginning and at the end of the section. Below, in the item **"Geometry and dynamics of the section",** for the same river (item 4.2.2.) is given the average flow velocity for the whole section. In the models is used the linear interpolation for the water flow rate equal to the product of the flow velocity by the cross-cross-section area (see paragraph 1.5). The flow velocity is calculated for each point of the section with account of the river width and depth, which can vary over a wide range within the section. Thus, if the cross-section area in the middle of the section is smaller, than at its ends, the flow velocity in the middle of the section, i.e. the average velocity on the whole section, will be higher than the flow velocity at the ends of the section.

Table 8.13. Initial data for pollution objects of the river Khobistskali: $N = 2$

j	Name	T_j	ξ_j	η_j	z_j
1	r. Ochkhomuri	∞	26500.000	100.0000	0.100000
2	r. Chznistskali	∞	44000.000	-100.0000	0.100000

Table 8.14. Initial data for upper section of the river Khobistskali: $N = 2$

j	Name	σ_j
1	NO3	1.100000
2	PO4	0.018000

Table 8.15. Initial data for capacities of pollution sources of the river Khobistskali: $N = 2$

$j \setminus k$	1: Expense	2: NO3	3: PO4
1: r. Ochkhomuri	1.000000	1.200000	0.010000
2: r. Chznistskali	8.000000	3.360000	0.051000

Table 8.16. Initial data for diffusion factors in the upper cross-section of the river Khobistskali: $N = 2$

j	Parameter	K_x	$K_x^{'}$	K_y	$K_y^{'}$	K_z	$K_z^{'}$
1	NO3	0.180000	0.185000	0.110000	0.115000	0.110000	0.115000
2	PO4	0.550000	0.555000	0.520000	0.525000	0.520000	0.525000

Table 8.17. Initial data for non-conservativity factors (in the upper) and self-clarification factors (in the lower) in the upper cross-section of the river Khobistskali: $N = 2$

j	Parameter	l_j	q_j
2	PO_4	1000.000	0.992000
	PO_4	1000.000	0.992000
j	Parameter	ζ_j	$\zeta_j^{'}$
2	NO_3	0	0
	PO_4	0	0

8.3.2. Calculation Results

8.3.2.1. The River Choga; One- and Two-Dimensional Models

Let's consider the transport of pollutants in the section of the river Choga between points 1 and 2 by one and two dimensional models. The river's characteristic data used for simulation of water pollution are the following.

Basic initial data

Type of the model: One- or two-dimensional;
Polluting substance: NO_3;
Boundary conditions on the lower section: Classical.

Accuracy of calculations

The total number of nodal points: $n = 1000\ (m = 1); n = 19992\ (m = 2);$

The number of nodal points along the Y-axis: $n_2 = 20\ (m = 2);$

The coefficient determining the step of time discretization: $c_t = 1.00000;$

The step of time discretization: $\tau = 22.0220\ (m = 1); \tau = 109.891 (m=2).$

Geometry and dynamics of the section

Length of the section: $L = 11000.0;$

Mean width of the river: $w = 7.00000$ ($m = 2$);

Mean flow velocity: $v = 0.68429$;

Mean water flow rate: $vE = 0.63966$;

Time of water renovation: $T = 4h \quad 27\,\text{min} \quad 0.75s$.

Water parameters

Mean diffusion factor: $K_x = 0.18350; \quad K_y = 0.11350$;

Mean non-conservativity factor: $\zeta = 0$;

Boundary conditions in the upper section: $\sigma = 3.78000$;

Zero value of concentration: $S = 0$;

Mean concentration: $s_0 = 4.02058$.

Calculation results: at $m = 1$.

Table 8.18. Concentrations for moment $t = 2h \quad 13\,\text{min} \quad 36.02s$; the number of steps $k = 108$

j	1	2	3	4	5	6	7	8	9	10
x_j	343.75	687.50	1031.3	1375.0	1718.8	2062.5	2406.3	2750.0	3093.8	3437.5
s_j	3.6980	3.6257	3.5667	3.4929	3.4160	3.3715	3.3032	3.2439	3.1953	3.1008

j	11	12	13	14	15	16	17	18	19	20
x_j	3781.3	4125.0	4468.8	4812.5	5156.3	5500.0	5843.8	6187.5	6531.3	6875.0
s_j	3.1575	3.2481	3.5244	0.9122	0.0923	0.0749	0.0705	0.0679	0.0677	0.0717

j	21	22	23	24	25	26	27	28	29	30
x_j	7218.8	7562.5	7906.3	8250.0	8593.8	8937.5	9281.3	9625.0	9968.8	1.03e4
s_j	0.0691	0.0621	0.0687	0.0727	0.0557	0.0500	0.0625	0.0573	0.0486	0.0589

j	31	32
x_j	1.06e4	1.10e4
s_j	0.0602	0.0499

Table 8.19. Concentrations for moment $t = 4h \;\; 27\min 12.03s$;

the number of steps $k = 216$

j	1	2	3	4	5	6	7	8	9	10
x_j	343.75	687.50	1031.3	1375.0	1718.8	2062.5	2406.3	2750.0	3093.8	3437.5
s_j	3.6981	3.6256	3.5665	3.4921	3.4148	3.3744	3.3067	3.2383	3.2025	3.1470

j	11	12	13	14	15	16	17	18	19	20
x_j	3781.3	4125.0	4468.8	4812.5	5156.3	5500.0	5843.8	6187.5	6531.3	6875.0
s_j	3.0912	3.0491	2.9989	2.9453	2.9104	2.8633	2.8125	2.7825	2.7377	2.6996

j	21	22	23	24	25	26	27	28	29	30
x_j	7218.8	7562.5	7906.3	8250.0	8593.8	8937.5	9281.3	9625.0	9968.8	1.03e4
s_j	2.6687	2.6268	2.5867	2.5733	2.5541	2.5327	2.5399	2.4587	2.1681	2.7883

j	31	32
x_j	1.06e4	1.10e4
s_j	1.3126	0.2572

Table 8.20. Concentrations for moment $t = 6h \;\; 40\min \;\; 48.05s$;

the number of steps: $k = 324$

j	1	2	3	4	5	6	7	8	9	10
x_j	343.75	687.50	1031.3	1375.0	1718.8	2062.5	2406.3	2750.0	3093.8	3437.5
s_j	3.6981	3.6256	3.5665	3.4921	3.4148	3.3744	3.3067	3.2383	3.2025	3.1470

j	11	12	13	14	15	16	17	18	19	20
x_j	3781.3	4125.0	4468.8	4812.5	5156.3	5500.0	5843.8	6187.5	6531.3	6875.0
s_j	3.0912	3.0490	2.9988	2.9454	2.9107	2.8637	2.8124	2.7808	2.7383	2.7013

j	21	22	23	24	25	26	27	28	29	30
x_j	7218.8	7562.5	7906.3	8250.0	8593.8	8937.5	9281.3	9625.0	9968.8	1.03e4
s_j	2.6655	2.6278	2.5977	2.5615	2.5224	2.4837	2.4632	2.4258	2.3937	2.3734

j	31	32
x_j	1.06e4	1.10e4
s_j	2.3422	2.3117

Table 8.21. Concentrations for moment $t = 8h \;\; 54\min \;\; 24.06s$;
the number of steps: $k = 432$

j	1	2	3	4	5	6	7	8	9	10
x_j	343.75	687.50	1031.3	1375.0	1718.8	2062.5	2406.3	2750.0	3093.8	3437.5
s_j	3.6981	3.6256	3.5665	3.4921	3.4148	3.3744	3.3067	3.2383	3.2025	3.1470

j	11	12	13	14	15	16	17	18	19	20
x_j	3781.3	4125.0	4468.8	4812.5	5156.3	5500.0	5843.8	6187.5	6531.3	6875.0
s_j	3.0912	3.0490	2.9988	2.9454	2.9107	2.8637	2.8124	2.7808	2.7383	2.7013

j	21	22	23	24	25	26	27	28	29	30
x_j	7218.8	7562.5	7906.3	8250.0	8593.8	8937.5	9281.3	9625.0	9968.8	1.03e4
s_j	2.6655	2.6278	2.5977	2.5615	2.5224	2.4836	2.4633	2.4258	2.3937	2.3734

j	31	32
x_j	1.06e4	1.10e4
s_j	2.3421	2.3116

Calculation results: at $m = 2$.

Table 8.22. Concentrations for moment $T = 2h \;\; 11\min 52.17s$;
the number of steps: $k = 72$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	343.75	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016
2	687.50	3.6164	3.6164	3.6164	3.6163	3.6163	3.6153	3.6163	3.6163
3	1031.3	3.5582	3.5583	3.5586	3.5590	3.5595	3.5957	3.5598	3.5596
4	1375.0	3.4891	3.4892	3.4892	3.4893	3.4893	3.4917	3.4894	3.4894
5	1718.8	3.4237	3.4237	3.4246	3.4237	3.4237	3.4238	3.4236	3.4236
6	2062.5	3.3665	3.3666	3.3922	3.3664	3.3659	3.3656	3.3654	3.3653
7	2406.3	3.3082	3.3082	3.3101	3.3082	3.3081	3.3082	3.3080	3.3080
8	2750.0	3.2358	3.2358	3.2359	3.2357	3.2356	3.2328	3.2356	3.2356
9	3093.8	3.1870	3.1871	3.1873	3.1876	3.1879	3.2096	3.1881	3.1880
10	3437.5	3.0894	3.0894	3.0895	3.0895	3.0895	3.0913	3.0896	3.0895
11	3781.3	2.8677	2.8677	2.8676	2.8677	2.8677	2.8679	2.8677	2.8677
12	4125.0	2.4469	2.4470	2.4631	2.4467	2.4464	2.4462	2.4460	2.4459
13	4468.8	1.8186	1.8186	1.8201	1.8185	1.8185	1.8182	1.8184	1.8184
14	4812.5	1.1698	1.1699	1.1701	1.1700	1.1702	1.1766	1.1702	1.1702

Table 8.22. (Continued)

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
15	5156.3	0.6554	0.6555	0.6557	0.6558	0.6561	0.6679	0.6562	0.6561
16	5500.0	0.3264	0.3264	0.3261	0.3265	0.3265	0.3278	0.3266	0.3266
17	5843.8	0.1658	0.1658	0.1689	0.1658	0.1657	0.1658	0.1657	0.1656
18	6187.5	0.1033	0.1034	0.1127	0.1032	0.1029	0.1027	0.1026	0.1025
19	6531.3	0.0734	0.0734	0.0744	0.0734	0.0733	0.0731	0.0732	0.0732
20	6875.0	0.0666	0.0666	0.0668	0.0667	0.0668	0.0726	0.0669	0.0668
21	7218.8	0.0684	0.0685	0.0686	0.0687	0.0689	0.0770	0.0690	0.0689
22	7562.5	0.0587	0.0587	0.0580	0.0588	0.0589	0.0599	0.0590	0.0590
23	7906.3	0.0618	0.0619	0.0700	0.0618	0.0616	0.0615	0.0613	0.0613
24	8250.0	0.0650	0.0650	0.0718	0.0649	0.0646	0.0645	0.0643	0.0642
25	8593.8	0.0604	0.0604	0.0613	0.0604	0.0603	0.0602	0.0603	0.0602
26	8937.5	0.0545	0.0545	0.0546	0.0544	0.0543	0.0504	0.0543	0.0543
27	9281.3	0.0601	0.0601	0.0601	0.0603	0.0604	0.0657	0.0605	0.0604
28	9625.0	0.0630	0.0630	0.0645	0.0630	0.0629	0.0636	0.0628	0.0628
29	9968.8	0.0477	0.0476	0.0286	0.0480	0.0484	0.0489	0.0490	0.0491
30	1.03e4	0.0605	0.0605	0.0650	0.0604	0.0602	0.0600	0.0599	0.0599
31	1.06e4	0.0569	0.0569	0.0575	0.0568	0.0568	0.0567	0.0567	0.0567
32	1.10e4	0.0532	0.0532	0.0533	0.0532	0.0532	0.0532	0.0531	0.0531

Table 8.23. Concentrations for moment $T = 4h \;\; 23\min \;\; 44.34s$ **;**
the number of steps: $k = 144$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	343.75	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016
5	1718.8	3.4237	3.4237	3.4246	3.4237	3.4236	3.4238	3.4236	3.4236
10	3437.5	3.1396	3.1397	3.1397	3.1397	3.1398	3.1416	3.1398	3.1398
15	5156.3	2.9044	2.9044	2.9046	2.9047	2.9050	2.9169	2.9051	2.9050
20	6875.0	2.6959	2.6959	2.6961	2.6961	2.6962	2.7019	2.6962	2.6962
25	8593.8	2.4449	2.4449	2.4458	2.4448	2.4448	2.4447	2.4447	2.4447
30	1.03e4	1.3551	1.3551	1.3595	1.3549	1.3547	1.3546	1.3545	1.3544
32	1.10e4	0.7895	0.7895	0.7896	0.7895	0.7895	0.7894	0.7894	0.7894

Table 8.24. Concentrations for moment $T = 6h \;\; 35\min \;\; 36.52s$ **;**
the number of steps: $k = 216$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	343.75	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016
5	1718.8	3.4237	3.4237	3.4246	3.4237	3.4236	3.4238	3.4236	3.4236
10	3437.5	3.1396	3.1397	3.1397	3.1397	3.1398	3.1416	3.1398	3.1398
15	5156.3	2.9044	2.9044	2.9046	2.9047	2.9050	2.9169	2.9051	2.9050
20	6875.0	2.6960	2.6960	2.6962	2.6961	2.6963	2.7020	2.6963	2.6962
25	8593.8	2.5210	2.5210	2.5218	2.5209	2.5209	2.5208	2.5208	2.5208
30	1.03e4	2.3719	2.3720	2.3764	2.3718	2.3716	2.3715	2.3713	2.3713
32	1.10e4	2.3103	2.3103	2.3104	2.3103	2.3102	2.3102	2.3102	2.3102

Table 8.25. Concentrations for moment $T = 8h \;\; 47\min \;\; 28.69s$; the number of steps: $k = 288$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	343.75	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016	3.7016
5	1718.8	3.4237	3.4237	3.4246	3.4237	3.4236	3.4238	3.4236	3.4236
10	3437.5	3.1396	3.1397	3.1397	3.1397	3.1398	3.1416	3.1398	3.1398
j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
15	5156.3	2.9044	2.9044	2.9046	2.9047	2.9050	2.9169	2.9051	2.9050
20	6875.0	2.6960	2.6960	2.6962	2.6961	2.6963	2.7020	2.6963	2.6962
25	8593.8	2.5210	2.5210	2.5218	2.5209	2.5209	2.5208	2.5208	2.5208
30	1.03e4	2.3719	2.3720	2.3764	2.3718	2.3716	2.3715	2.3713	2.3713
32	1.10e4	2.3103	2.3103	2.3104	2.3103	2.3102	2.3102	2.3102	2.3102

8.3.22. The River Khobistskali; One- and Two-Dimensional Models

In this paragraph is offered the results of simulation of pollutants transport in the section of the Khobistskali between points 3 and 4 by one- and two-dimensional models. The characteristic data of the river used for simulation of water pollution are the following.

Basic initial data

Type of the model: One- or two-dimensional;
Polluting substance: PO4;
Boundary conditions on the lower section: Classical.

Accuracy of calculations

The total number of nodal points: $n = 1000 \;(m = 1); n = 19992 \;(m = 2);$

The number of nodal points along the Y -axis: $n_2 = 20 \;\; (m = 2)$;

The coefficient determining the step of time discretization: $c_t = 1.00000$;

The step of time discretization: $\tau = 89.6897 \;(m = 1); \tau = 1 \;\; 147.44 \;(m = 2).$

Geometry and dynamics of the section

Length of the section: $L = 44800.0$;

Mean width of the river: $w = 57.8268 \;(m = 2)$;

Mean flow velocity: $v = 1.08368$; (see note in the item 4.1.2)

Mean water flow rate: $vE = 41.8975$;

Time of water renovation: $T = 11h \;\; 22\min \;\; 41.16s$.

Water parameters

Mean diffusion factor: $K_x = 0.55250; \;\; K_y = 0.52250$;

Mean non-conservativity factor: $\zeta = 0$;

Boundary conditions in the upper section: $\sigma = 0.01800$;

Zero value of concentration: $S = 0$;

Mean concentration: $s_0 = 0.04318$.

Calculation results: at $m = 1$.

Table 8.26. Concentrations for moment $t = 5h \;\; 40\min \;\; 49.25s$; the number of steps: $k = 228$

j	1	2	3	4	5	6	7	8	9	10
x_j	1400.0	2800.0	4200.0	5600.0	7000.0	8400.0	9800.0	1.12e4	1.26e4	1.40e4
s_j	0.0164	0.0151	0.0140	0.0131	0.0123	0.0113	0.0111	0.0100	0.0091	0.0109

j	11	12	13	14	15	16	17	18	19	20
x_j	1.54e4	1.68e4	1.82e4	1.96e4	2.10e4	2.24e4	2.38e4	2.52e4	2.66e4	2.80e4
s_j	0.0018	4.2e-5	1.5e-5	1.7e-6	-3.1e-5	-3.1e-5	2.4e-5	0.0001	8.7e-5	2.5e-5

j	21	22	23	24	25	26	27	28	29	30
x_j	2.94e4	3.08e4	3.22e4	3.36e4	3.50e4	3.64e4	3.78e4	3.92e4	4.06e4	4.20e4
s_j	1.1e-5	9.7e-5	0.0002	0.0001	-0.0001	-0.0002	0.0001	0.0006	0.0003	-0.0004

j	31	32
x_j	4.34e4	4.48e4
s_j	-0.0010	0.0016

Table 8.27. Concentrations for moment

$t = 11h \;\; 21\min \;\; 38.50s$; **the number of steps:** $k = 456$

j	1	2	3	4	5	6	7	8	9	10
x_j	1400.0	2800.0	4200.0	5600.0	7000.0	8400.0	9800.0	1.12e4	1.26e4	1.40e4
s_j	0.0164	0.0151	0.0140	0.0130	0.0122	0.0115	0.0108	0.0102	0.0097	0.0092

j	11	12	13	14	15	16	17	18	19	20
x_j	1.54e4	1.68e4	1.82e4	1.96e4	2.10e4	2.24e4	2.38e4	2.52e4	2.66e4	2.80e4
s_j	0.0088	0.0084	0.0081	0.0077	0.0073	0.0071	0.0069	0.0068	0.0065	0.0061

Table 8.27. (Continued)

j	21	22	23	24	25	26	27	28	29	30
x_j	2.94e4	3.08e4	3.22e4	3.36e4	3.50e4	3.64e4	3.78e4	3.92e4	4.06e4	4.20e4
s_j	0.0059	0.0060	0.0061	0.0053	0.0052	0.0050	0.0059	0.0035	0.0012	-0.0002

j	31	32
x_j	4.34e4	-0.0010
s_j	4.48e4	0.0016

Table 8.28. Concentrations for moment $t = 17h \;\; 02\min \;\; 27.75s$; the number of steps: $k = 684$;

j	1	2	3	4	5	6	7	8	9	10
x_j	1400.0	2800.0	4200.0	5600.0	7000.0	8400.0	9800.0	1.12e4	1.26e4	1.40e4
s_j	0.0164	0.0151	0.0140	0.0130	0.0122	0.0115	0.0108	0.0102	0.0097	0.0092

j	11	12	13	14	15	16	17	18	19	20
x_j	1.54e4	1.68e4	1.82e4	1.96e4	2.10e4	2.24e4	2.38e4	2.52e4	2.66e4	2.80e4
s_j	0.0088	0.0084	0.0081	0.0077	0.0074	0.0071	0.0069	0.0067	0.0065	0.0062

j	21	22	23	24	25	26	27	28	29	30
x_j	2.94e4	3.08e4	3.22e4	3.36e4	3.50e4	3.64e4	3.78e4	3.92e4	4.06e4	4.20e4
s_j	0.0060	0.0059	0.0059	0.0056	0.0052	0.0050	0.0051	0.0055	0.0051	0.0043

j	31	32
x_j	4.34e4	4.48e4
s_j	0.0036	0.0060

Table 8.29. Concentrations for moment $t = 22h \;\; 43\min \;\; 17.00s$; the number of steps: $k = 912$

j	1	2	3	4	5	6	7	8	9	10
x_j	1400.0	2800.0	4200.0	5600.0	7000.0	8400.0	9800.0	1.12e4	1.26e4	1.40e4

s_j	0.0164	0.0151	0.0140	0.0130	0.0122	0.0115	0.0108	0.0102	0.0097	0.0092

Table 8.29. (Continued)

j	11	12	13	14	15	16	17	18	19	20
x_j	1.54e4	1.68e4	1.82e4	1.96e4	2.10e4	2.24e4	2.38e4	2.52e4	2.66e4	2.80e4
s_j	0.0088	0.0084	0.0081	0.0077	0.0074	0.0071	0.0069	0.0067	0.0065	0.0062

j	21	22	23	24	25	26	27	28	29	30
x_j	2.94e4	3.08e4	3.22e4	3.36e4	3.50e4	3.64e4	3.78e4	3.92e4	4.06e4	4.20e4
s_j	0.0060	0.0059	0.0059	0.0056	0.0052	0.0050	0.0051	0.0055	0.0051	0.0043

j	31	32
x_j	4.34e4	4.48e4
s_j	0.0036	0.0060

Calculation results: at $m = 2$.

Table 8.30. Concentrations for moment $t = 5h \;\; 05\min \;\; 58.97s$;
the number of steps: $k = 16$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	1400.0	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164
5	7000.0	0.0113	0.0113	0.0113	0.0113	0.0113	0.0113	0.0113	0.0113
10	1.40e4	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029
15	2.10e4	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
20	2.80e4	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
25	3.50e4	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
30	4.20e4	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0001	0.0001
32	4.48e4	0.0027	0.0021	0.0018	0.0016	0.0015	0.0013	0.0013	0.0012

Table 8.31. Concentrations for moment $t = 10h \;\; 11\min \;\; 57.94s$;
the number of steps: $k = 32$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	1400.0	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164
5	7000.0	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122
6	8400.0	0.0115	0.0115	0.0115	0.0115	0.0115	0.0115	0.0115	0.0115
7	9800.0	0.0108	0.0108	0.0108	0.0108	0.0108	0.0108	0.0108	0.0108
8	1.12e4	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102
9	1.26e4	0.0097	0.0097	0.0097	0.0097	0.0097	0.0097	0.0097	0.0097
10	1.40e4	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092
15	2.10e4	0.0069	0.0069	0.0069	0.0069	0.0069	0.0069	0.0069	0.0069
20	2.80e4	0.0044	0.0044	0.0044	0.0044	0.0044	0.0045	0.0045	0.0045

25	3.50e4	0.0020	0.0020	0.0020	0.0020	0.0020	0.0020	0.0021	0.0021
30	4.20e4	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002
32	4.48e4	0.0025	0.0025	0.0023	0.0021	0.0019	0.0017	0.0017	0.0016

Table 8.32. Concentrations for moment $t = 15h \;\; 17\min \;\; 56.91s$; the number of steps: $k = 48$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	1400.0	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164
5	7000.0	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122
10	1.40e4	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092
15	2.10e4	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
20	2.80e4	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064
25	3.50e4	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054
30	4.20e4	0.0037	0.0037	0.0037	0.0038	0.0038	0.0038	0.0039	0.0039
32	4.48e4	0.0064	0.0060	0.0058	0.0056	0.0054	0.0053	0.0052	0.0051

Table 8.33. Concentrations for moment $t = 20h \;\; 23\min \;\; 55.88s$; the number of steps: $k = 64$

j	x_j	s_{1j}	s_{2j}	s_{3j}	s_{4j}	s_{5j}	s_{6j}	s_{7j}	s_{8j}
1	1400.0	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164	0.0164
5	7000.0	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122	0.0122
10	1.40e4	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092	0.0092
15	2.10e4	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
20	2.80e4	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064	0.0064
25	3.50e4	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054
30	4.20e4	0.0039	0.0040	0.0040	0.0041	0.0041	0.0041	0.0041	0.0042
32	4.48e4	0.0067	0.0065	0.0063	0.0061	0.0059	0.0058	0.0057	0.0057

8.3.3. Results of Modeling and Discussion

The above computations were carried out on the needs of the Ministry of Agriculture of Georgia, which was interested in the estimation of the effect of agricultural fields on the pollution level of the considered rivers. As the River Choga becomes polluted only by these pollution sources, at modeling actually all pollution sources were taken into account. Whereas at modeling the pollution of the River Khobistskali was taken into account the pollution brought in the river only the Ochkhomuri and the Chanistskali, because it is rather difficult to take into account all the pollution sources of the given river. By the difference between the measured and the simulated values of controlled components in the sections of the river, was estimated the effect of agricultural fields located along the banks of the river in the interval between two sections on the pollution degree of the Khobistskali (see below). In this sense, the example is schematic, as the number, the arrangement and the capacities of pollution sources of the River Khobistskali partially correspond to the real situation. Though, the geometry of the rivers, the arrangement of control sections, the concentrations of polluting

substances in the rivers completely correspond to the real data. The constantly operating pollution sources on the River Choga are considered.

The results of modeling of the pollution of the River Choga for the NO_3 component, and the River Khobistskali – for the PO_4 component, are given above. The modeling was carried out with the help of one-, two- and three-dimensional models. Due to the river dimensions, the results of two- and three-dimensional models practically coincide. Therefore, below are discussed only the results of one- and two-dimensional models. The results of modeling allow the following conclusions.

One-dimensional model. The River Choga (Figure 8.2). Because of the effect of unpolluted underground waters on the River Choga, which is taken into account in the model as a water source evenly distributed along its full length of the river, the concentration of NO_3 component in the upper section of the River Choga decreases to 3.698 from 3.78 mg/l through 343.75 m, and through 687.5 m it decreases to 3.6257 mg/l. At the distance of 1000 m from the upper cross-section, the first pollution source operates. Under the effect of this source, the rate of reduction of the pollutant concentration decreases at the cost of dilution and at the distance 1031.3 m from the upper cross-section, the concentration becomes equal to 3.5667 mg/l. Really, along the first 343.75 m, the concentration of NO_3 in the river water decreases by 0,082 mg/l, along the following 343.75 m it decreases by 0.0723 mg/l, and along the following 343.75 m it decreases by 0.059 mg/l, because on this section the pollution source operates. This pollution source could not affect more considerably the river water, as the volume of water from each source is less by a factor of ≈ 42.6 than the volume of water in the river, and the concentration of the polluting substance is also less than the pollution of the river by a factor of 5. A similar effect of nine other equidistant sources of pollution is observed along the full length of the river. In ≈ 2 h and 13 minutes, the pollution from the upper section of the river spreads at the distance of 4 500 - 4 800 m. Then the level of pollution in the river sharply falls because of their insignificant capacity the sources of pollution located below, do not render appreciable influence on the river. In ≈ 4 h and 27 minutes the pollution from the upper section reaches the points located at the distance of 10 000 m, though the concentration appears, reduced by a factor of ≈ 1.359 due to the effect of unpolluted underground waters and at the expense of total increase in the water flow rate in the river. In ≈ 6 h h and 40 minutes, at the distance of 11 000 m the pollution is less by a factor of ≈ 1.635 than in the upper section (at the expense of the noted factor), and further the distribution of the pollution in the river remains practically at the same level, i.e. the process of pollution reaches the steady state (see the results of computation in ≈ 8 h and 54 minutes).

Because the pollution sources are spaced widely (at 1000 m) and their influence on the river is weak enough (the volume of waste waters and the pollution level are small in comparison with the river). On the other hand, the increase in the water flow rate of the river is significant enough, the effect of these sources on the river is not accumulated (i.e. the total effect is not tangible), since at the distance of 1000 m, at the expense of the above

mentioned, in the river the pollution level brought in not only by a pollution source, but also from the upper section, decreases to the minimum level.

The computation results for the **two-dimensional model (Figure 8.3)** practically coincide with the results for the one-dimensional model. Though the reduction of the concentration of the polluting substance in the lower section of the river, due to not reaching of the pollution from the upper section to the lower part of the river 2 h and 11 minutes occurs more smoothly than in the case of the one-dimensional model (see the results of computations for the two-dimensional model at $j = 11 \div 14$). On the basis of the analysis of the computation results for the two-dimensional model we can conclude that, for the river with the geometry similar to that of the Choga, the use of the two-dimensional model is unnecessary (concentrations calculated across the width of the river are practically identical). The computing results for the **three-dimensional** model practically do not differ from the two-dimensional model. Therefore, here we do not dwell on it.

The measured values of the concentration of NO_3 in the first and the second control sections of the River Choga (see Figure 8.2) are equal to 3.7 mg/l and 2.44 mg/l, respectively, and the values calculated by the model in the same sections are equal to: by the one-dimensional model – 3.698 mg/l and 2.342 mg/l; by the two- dimensional model – 3.7 mg/l and 2.31 mg/l. By simple comparison of the measured values and the values obtained by modeling, we are easily convinced in high quality of the modeling results as the relative error of the worst result (the two-dimensional model in the second section) is less than 5.6 %.

One-dimensional model. The River Khobistskali (Figure 8.4). A similar law is observed for the River Khobistskali by PO_4 parameter. In 5 h and 40 minutes the effect of the upper section is distributed downstream at the distance of 15 400 m ($j = 11$), in 11 h and 21 minutes the effect is distributed at the distance of $\approx 40\ 000$ m ($j = 29$). The influence of the Ochkhomuri on the Khobistskali is not tangible because of small quantity of water in the Ochkhomuri (less than in the Khobistskali by a factor of ≈ 42), the pollution level also is less than in the Khobistskali (0.01 mg/l – the Ochkhomuri; 0.018 mg/l – the Khobistskali). The influence of the Chanistskali is appreciable until the pollution from the upper section of the Khobistskali reaches the place of their confluence (see $t = 11$ h and 21 minutes). After the pollution from the upper section of the Khobistskali reaches the place of confluence of the Chanistskali, the influence of the latter is not tangible any more, because of the insignificant volume of water in it (less by a factor of $\approx 5{,}2$) and a rather low level of pollution (0.051 mg/l – the Chanistskali; 0.018 mg/l – the Khobistskali). See calculation results at $t = 17$ h and 02 minutes and $t = 22$ h and 43 minutes.

The application of **two- and three-dimensional models (Figure 8.5)** for such a river, as the Khobistskali is, at consideration of the section of the length at ≈ 45 km and two pollution sources, located at the places of confluence of the Rivers Ochkhomuri and Chaniststkali, makes no sense since the calculation results of two- and three-dimensional models practically coincide with the one-dimensional model and are identical across the width and in the depth of the river. As was mentioned above, by the difference between the

measured and simulated values of the controlled components in the sections of the river of our interest, there was estimated the degree of the influence of the agricultural fields located along of the river banks in the interval between two sections on the pollution of the River Khobistskali. The results of calculations showed that in 2002 from agricultural fields 566.4 kg NO_3 and 4.18 kg PO_4, act in the River Choga whereas in 2003 the amounts of the same pollutants were 276.4 kg and 3.17 kg, respectively. In 2002 the River Khobistskali got 62.8 tons NO_3 and 673.5 kg PO_4, and in 2003 got 43.6 tons NO_3 and 562.7 kg PO_4 respectively. Such reduction of the pollution level in 2003 in comparison with 2002 was basically caused by large-scale introduction of new environment friendly technologies in the agriculture in the Khobistskali basin with the financial support of the World Bank.

On the peculiarities of taking into account of pollution sources. In the considered models it was supposed that the considered section of the river contains constantly operating point sources of pollution. It means that the non-uniform parts of the diffusion equation under consideration contain impulse functions being linear combinations of Dirac deltas – functions. These functions and their derivatives are not limited therefore, in the vicinities of points of action of pollution sources, the difference schemes of the solution of the diffusion equations are not correct, which causes sharp oscillations of the obtained solutions, which are visible in Figure 8.2 – 8.5.

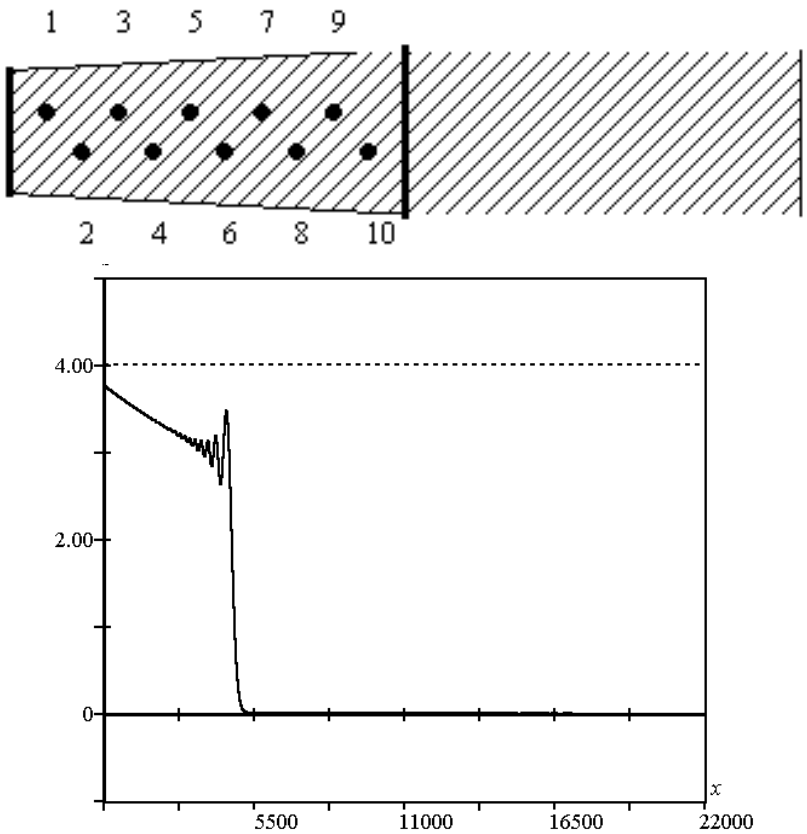
For elimination of this drawback, in the package is realized an approach described in paragraph 2.7, in which delta-function $\delta(x-a)$ is replaced by continuously-differentiated function $D(\varepsilon, x-a)$. It means that the point sources are replaced by extended sources, the capacity of each of which has the maximum corresponding to the capacity of the source at the point of its location. It is possible to name such sources as *quasi- pointwise*.

In the diagrams, similar to the ones shown in Figure 8.2 – 8.2, constructed for the given models of discharge of polluting components, oscillations of the obtained solutions are smoothed, as more considerably as the larger are the specified values of parameters ε and ν, i.e. the smoother are the functions of discharge, the more accurate are the results of the solution of the equations in the vicinities of the points of discharge.

About the accuracy of calculations. At computation of the concentration of polluting substances by the one-dimensional model, the accuracy of calculation was determined by setting number of central points along the full length of the river (11 000 m of the Choga) equal to 1 000, and at calculation by the two-dimensional model the total number of central points was equal to 20 000 (1 000 along the length of the river and 20 across the width of the river). Let's compare some concentrations of polluting substances calculated in these conditions from the Tables presented above for the river Choga. For example, compare the computed concentrations obtained with the help of the one- and two-dimensional models at the distance from the upper section equal to 343.75 m ($j=1$), 3781.3 m ($j=11$) and 10 600 m ($j=31$). The corresponding concentrations obtained with the help of the one-dimensional model are equal to 3.6980 mg/l, 3.1575 mg/l and 0.0602 mg/l; and with the help of the two-dimensional model – to 3.7016 mg/l, 2.8677 mg/l, 0.0569 mg/l.

The relative differences among these values are equal to 0,00097, 0,09178 and 0,0548, respectively. Thus, for the first point we obtained the relative difference between the calculation results by the one- and the two-dimensional models – 0,097 %, for the second point – 9,178 % and for the third point – 5,48 %. In our opinion, there is good agreement between the results for chosen accuracies of computation, as the step of time sampling was chosen so that the accuracy of the algorithm by the temporal coordinate approximately coincided with the accuracy of the algorithm by the spatial coordinates. The accuracy of concurrence of the models of different dimensionality is improved at increasing accuracy of the computation both by the spatial and temporal coordinates.

The hatched zones on the first line (here and below on the other figures) show the river bed with pollution sources (the black dots with numbers). The first zone (between two vertical lines) corresponds to the modeling cross-section of the river. The second zone corresponds to the classical boundary condition.



a) $t =$ 2 h 13 min 36.02 s.

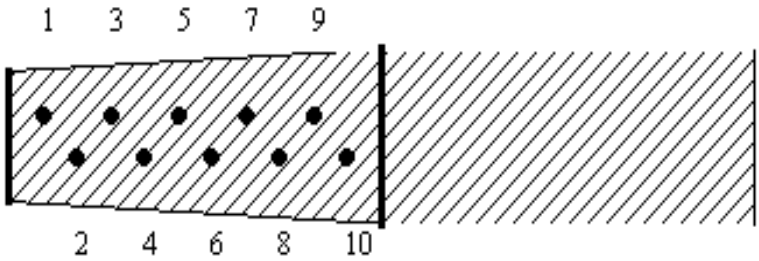
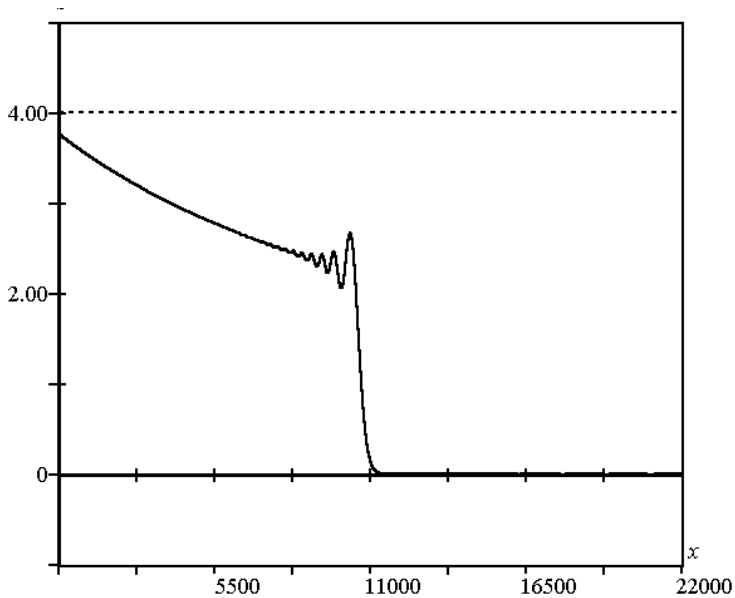
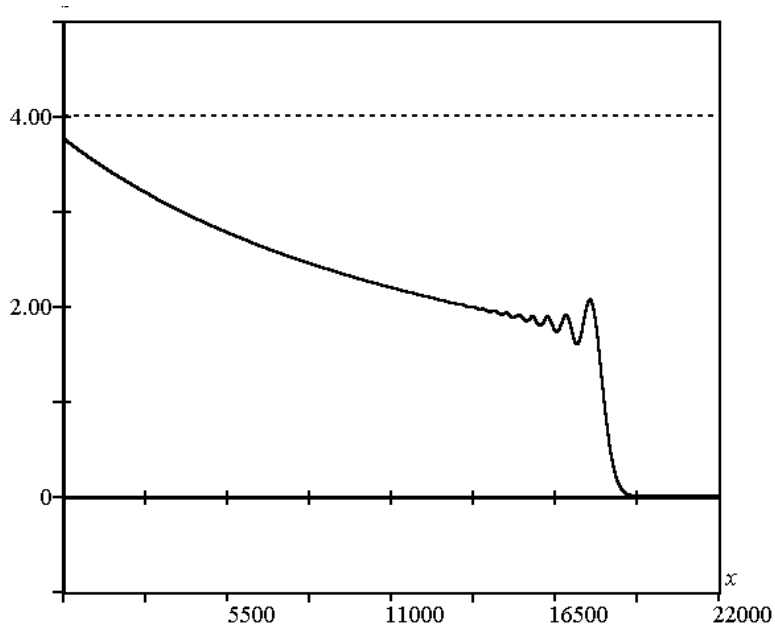


Figure 8.2. (Continued).

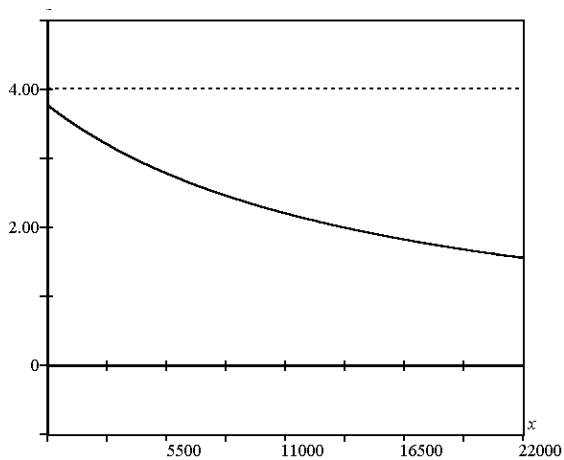


b) $t =$ 4 h 27 min 12.03 s.



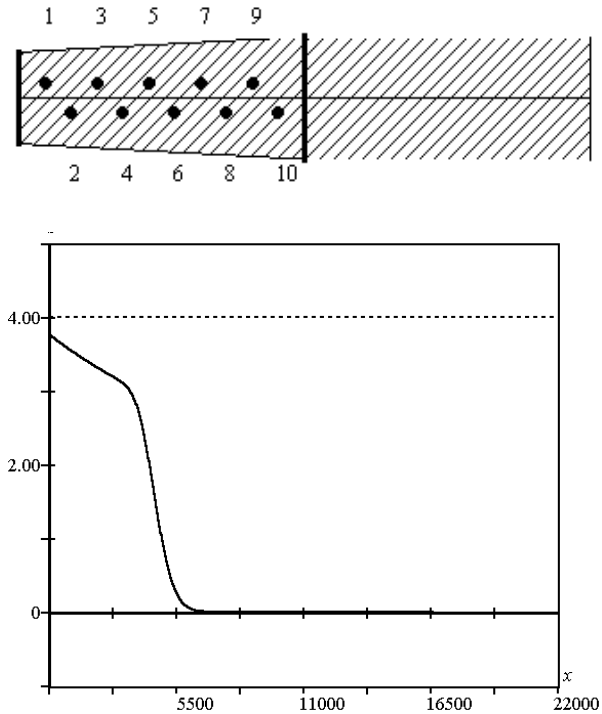
c) $t =$ 6 h 40 min 48.05 s.

Figure 8.2. (Continued).



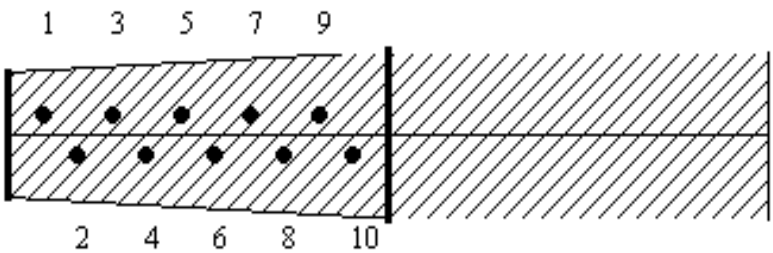
d) $t =$ 8 h 54 min 24.06 s.

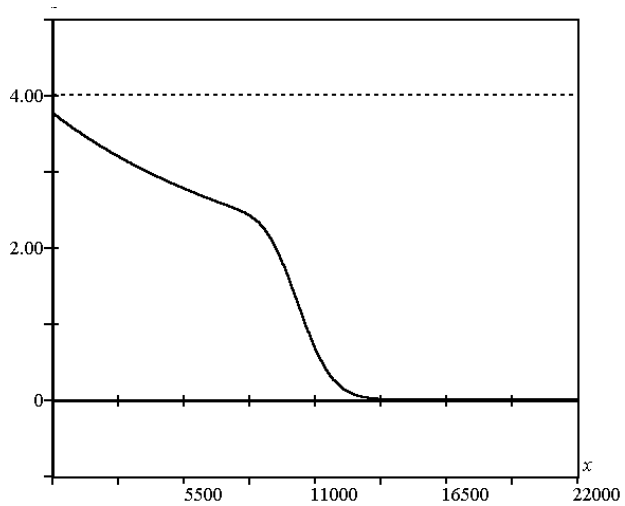
Figure 8.2. Plots of concentration of polluting substance in the river Choga depending from longitudinal coordinate ξ at 1D model.



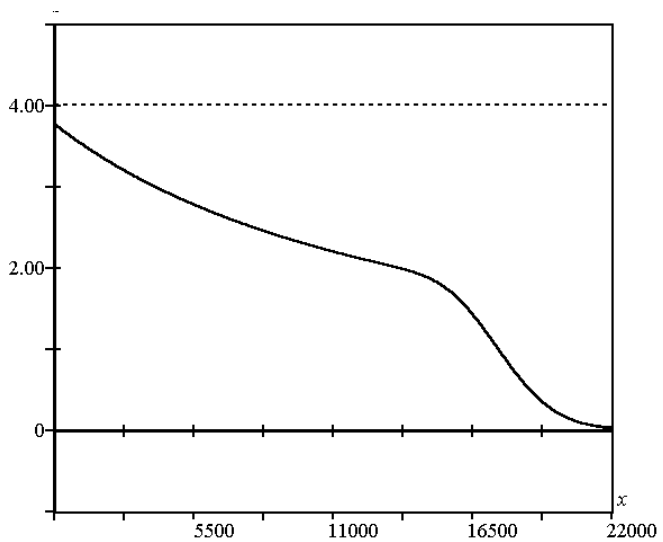
a) $t = 2$ h 11 min 52.17 s.

Figure 8.3. (Continued).



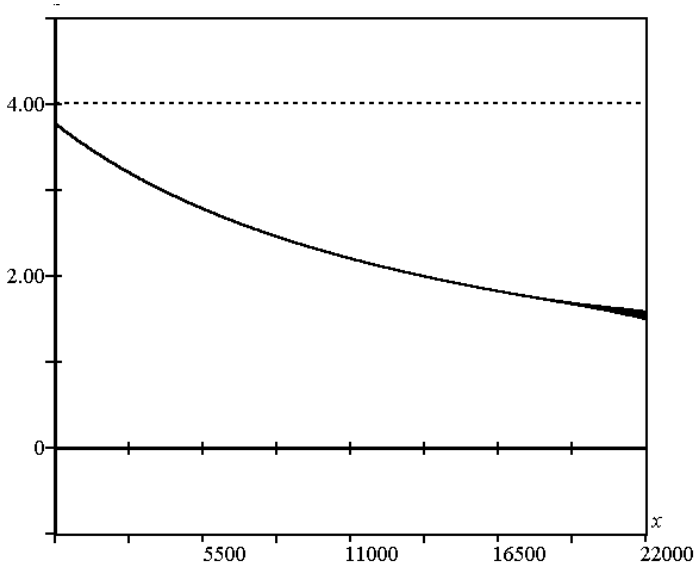


b) $t = 4$ h 23 min 44.34 s.



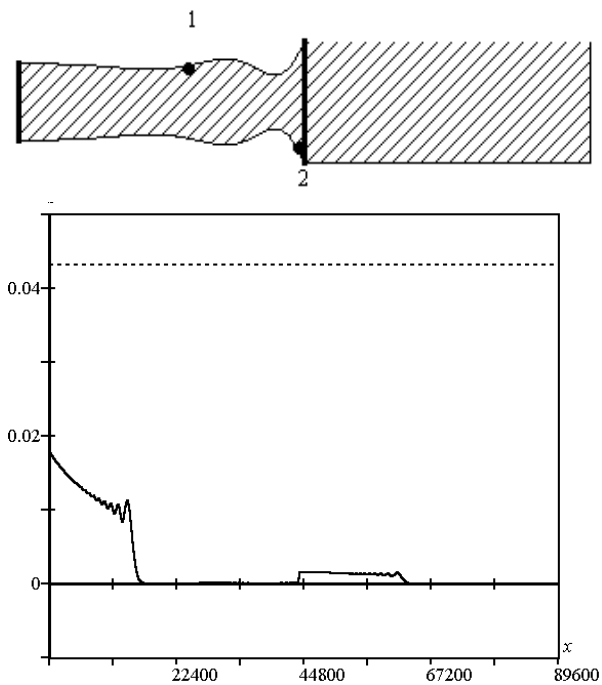
c) $t = 6$ h 35 min 36.52 s.

Figure 8.3. (Continued).



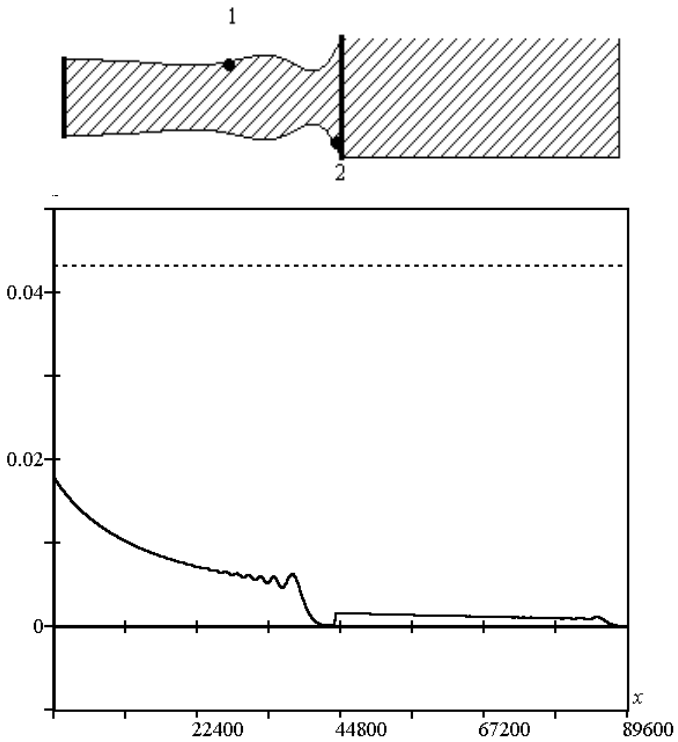
d) $t =$ 8 h 47 min 28.69 s.

Figure 8.3. Plots of concentration of polluting substance in the river Choga depending from longitudinal ξ at 2D model.

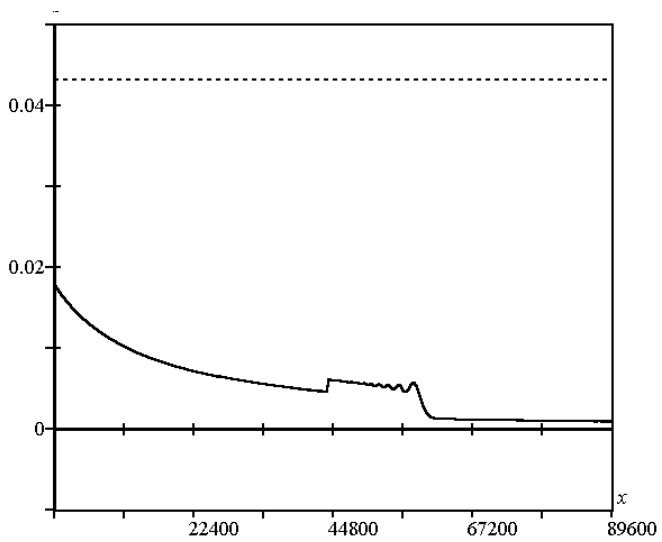


a) $t =$ 5 h 40 min 49.25 s.

Figure 8.4. (Continued).

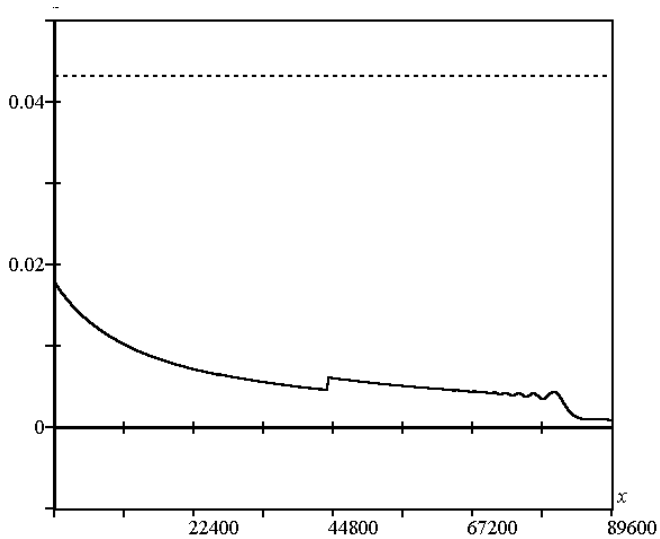


b) $t =$ 11 h 21 min 38.50 s.



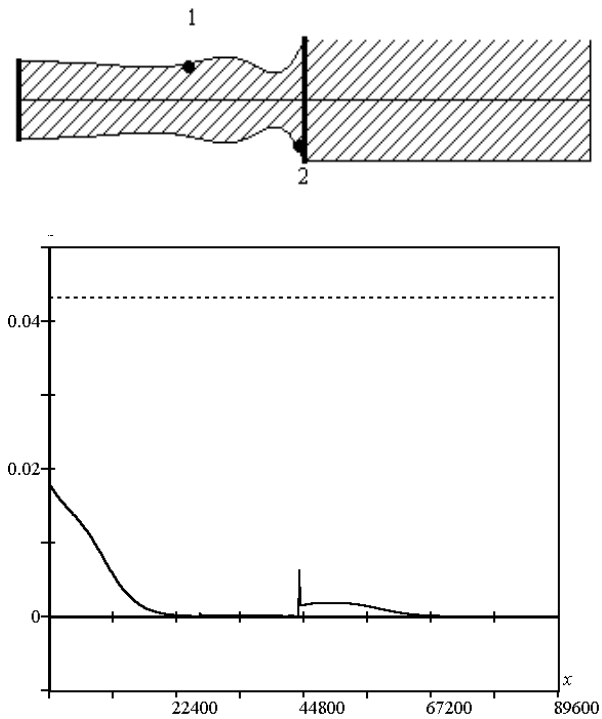
c) $t =$ 17 h 02 min 27.75 s.

Figure 8.4. (Continued).



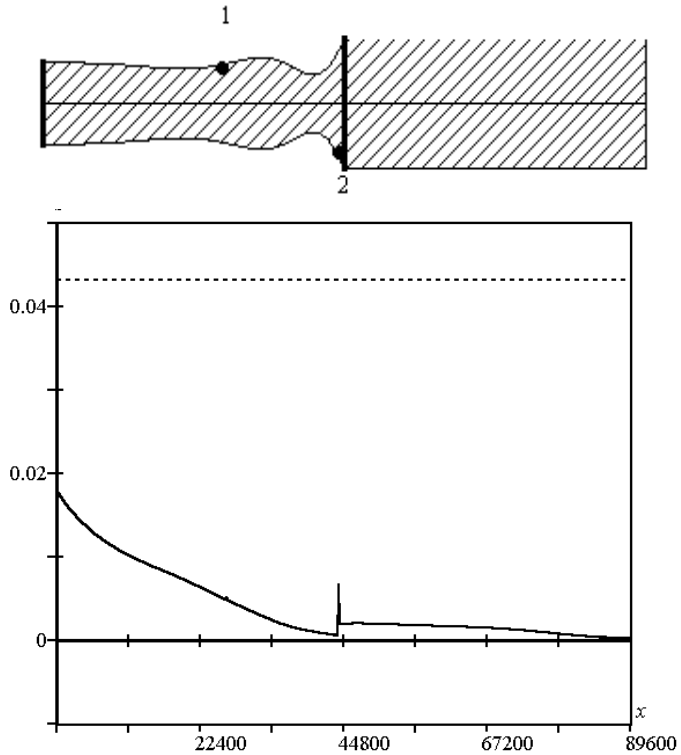
d) $t = 22$ h 43 min 17.00 s.

Figure 8.4. Plots of concentration of polluting substance in the river Khobi depending from longitudinal coordinate ξ at 1D model.

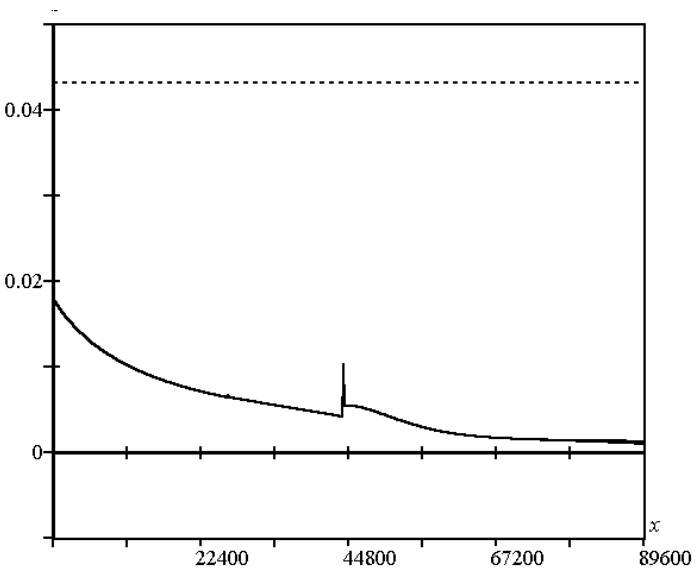


a) $t = 5$ h 05 min 58.97 s.

Figure 8.5. (Continued).

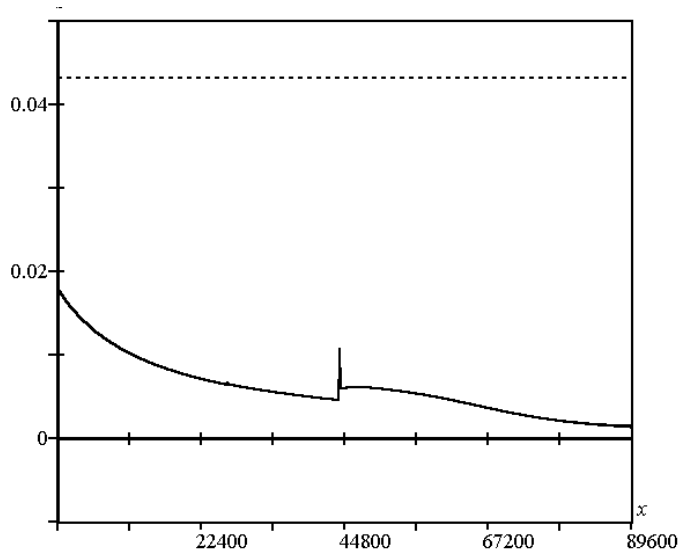


b) $t =$ 10 h 11 min 57.94 s.



c) $t =$ 15 h 17 min 56.91 s.

Figure 8.5. (Continued).



d) $t =$ 20 h 23 min 55.88 s.

Figure 8.5. Plots of concentration of polluting substance in the river Khobistskali depending from longitudinal coordinate ξ at 2D model.

8.4. River Pollution Components Mean Annual Values Estimation by Computer Modeling

With the help of described in Chapter 6 software of mathematical models of transport of pollution substances in the rivers we have carried out computation of quantities of polluting components dropped for 2002 and 2003 from pollution sources on separate sections of rivers the Choga, The Ochlhomuri, the Chanistskali and the Khobistskali, among cross-sections, included in the monitoring. On Figure 8.6 by red triangles are marked the monitoring cross-sections dividing the rivers as sections. By the help of these meanings we can: 1) to estimate a share working on each of section of the river of pollution sources in total amount of pollution of the river; 2) to estimate a change dropped for 2002, 2003 of quantities of polluting components on separate sections of the river, i.e. the efficiency of those measures which were carried out in these years on the marked pollution sources; 3) within the framework of those opportunities which are given by division of the rivers into sections by existing control cross-sections of monitoring, from each other to divide working on the river agricultural and others (for example, cities, located on the rivers; run other rivers) pollution sources; 4) to estimate the ecological load on the river from agricultural fields and cattle-breeding farms.

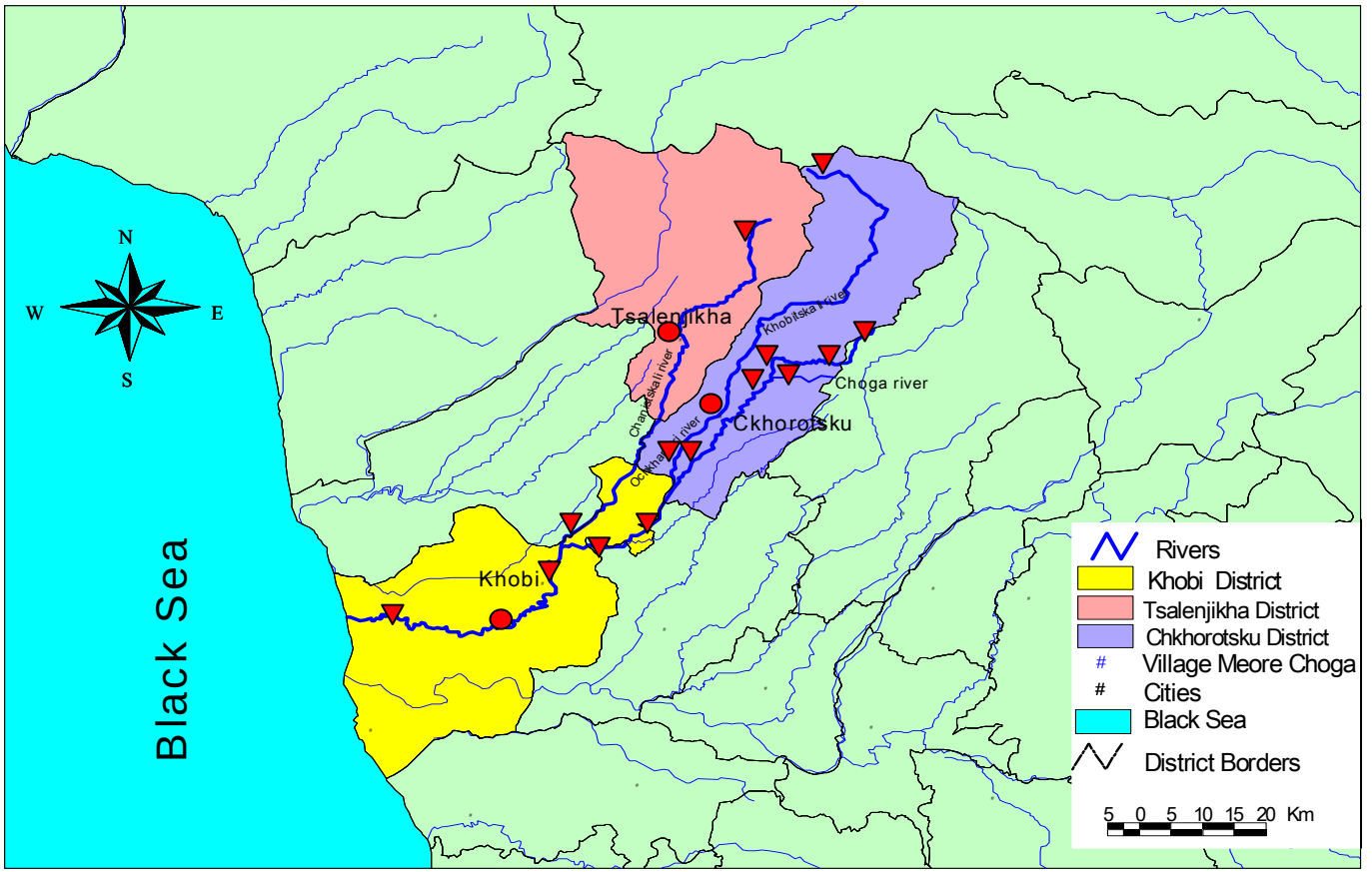


Figure 8.6. The river Khobistskali's basin with control sections.

Let us bring the brief description of the obtained results.

Modelling have carried out by basic biological parameters, nitrates (NO_3) and phosphates (PO_4), outgoing from agricultural fields and cattle-breeding farms. The results of monitoring of 2002 and 2003 were used for modelling. The idea of modelling consists in the following. On the basis of the monitoring results are known the mean annual concentrations of the marked components in each control cross-sections of the rivers. If we admit that on the given section of the river the pollution sources do not work, then existing in the top cross-section of the river the pollution level should decrease in the bottom cross-section at the expense of proceeding in the river of natural processes and ability of self purification. In reality for the Khobistskali's basin rivers this fact does not take place, as on each section of the river the appropriate pollution sources work. Therefore, if with the help of the developed mathematical models, we shall compute the concentration of polluting components in the bottom cross-section of the river by existing concentration in the top cross-section and after a condition that on this section of the river does not work any pollution source except of other river (if such runs in it on this section), then with a difference between measured and computed concentrations we shall easily compute the quantity of polluting components dropped in the river from pollution sources worked on this section.

In considered concrete case for modelling was used one-dimensional mathematical model of diffusion and transfer of pollution (see paragraph 1.2) [1, 5, 42]. It is caused by the following circumstances: in first, on the geometrical sizes of the considered rivers (in a case, when length of that section of the river, which modelling is carried out, 10 times and more surpass its width, to provide width is not meaningful because of full mixing of water of the river on a considered section of the river; also, if width of the river 10 and more time surpasses its depth, for the same reason, the account of depth loses of sense [5]), and in second because the average year data are used and the accuracy of model more high rank, in this case, loses of sense. The modelling results obtained by us for the Khobistskali's basin rivers with the help of one, two and three dimensional models, precisely have confirmed the marked reason. I.e. two and three dimensional models on all width and depth were given identical results with one-dimensional model that completely corresponds to the above – mentioned.

The concentrations of NO_3 and PO_4 on all the lengths of the rivers Choga, Ochkhomuri, Chanistskali and Khobistskali are calculated through the identical spatial steps. In case of the river Choga the length of the step is equal to 343,75 meters, in case of the r. Ochkhomuri the length of the step is equal to 1334,4 meters, in case of the r. Chanistskali the length of the step is equal to 1165,6 meters, and in case of the r. Khobistskali the length of the step is equal to 2337,5 meters. For the r. Choga the time of full updating of water, i.e. that time, which is necessary for run of water from a source of the river up to its confluence in other river, is equal to $\approx$15 h 36 min. For the rivers Ochkhomuri, Chanistskali and Khobistskali this time are accordingly equalled to $\approx$39 h 12 min, $\approx$20 h 25 min, $\approx$9 h 27 min. Therefore, at modelling on time parameter of the river through the appropriate interval of time it is possible taking of computed meaning of concentration in any point of the river on all length, as it corresponds to the counted by the appropriate model meaning of concentration in initial section.

In the tables 8.34, 8.35, 8.36, 8.37 are given the results of calculation of mean annual meanings of pollutants got from the appropriate sources in separate sections of the rivers during 2002, 2003.

The computation of mean annual meanings of pollutants dropped in the given section from above located pollution sources carried out as follows

$$S_{year}(kg/year)=(S_{mes}-S_{\mathrm{mod}})(mg/\sec)\,vE(m^3/\sec)\,60(\sec)\,24(hour)\cdot 365(day), \qquad (8.1)$$

where S_{year} is mean annual quantity of a polluting component dropped in the given section of the river from sources working on this section;

S_{mes} is measured mean annual meaning of concentration of a polluting component on the appropriate section;

S_{mod} is mean annual meaning of concentration of a polluting component computed by the model on the appropriate section;

vE is the charge of water in the appropriate section of the river.

The results of computation by formulae (8.1) are given in the tables 8.34, 8.35, 8.36 and 8.37. In the two last column of the tables are given by the considered rivers brought mean annual volumes of polluting components in places of them confluence, calculated as by directly results of measurement, and by direct summation of the computed by model the appropriate meanings in separate sections of the rivers. On the basis of these results is concluded:

- In 2002, 2003 r. Choga basically was polluted at sources by parameter NO_3, up to first section. In 2002 the river was polluted in more to bottom part by parameter PO_4, i.e. between the first and second sections. In 2003 the situation has changed and the river was polluted more up to the first section by parameter PO_4. The pollution of the river by both considered parameters in 2003 is significant decrease after comparison with 2002: by parameter NO_3 from 566,4 ton/years till 276,4 ton/years (≈ 2 times), and by parameter PO_4 from 4,18 kg/years till 3,17 kg/years ($\approx 1{,}32$ times). A difference between measured and computed meanings defined by mean annual volumes of the polluting components brought by the river Choga in the r. Ochkhomuri, on our sight, specifies high quality of modelling, if we take into account that circumstance that the modelling was carried out on the basis of the defective initial data (because of absence of the better). For example, expenses of the river (as well as for other rivers of the Khobistskali's basin) completely was measured only in 2003 (in 2002 only three times were measured the water expenses); exactly are not known the coefficients of diffusion and non conservative etc. Despite of told the modelling and measurement results with acceptable accuracy coincide with each other that specifies accuracy of the used technique.
- The pollution of the river Ochkhomuri by parameter NO_3 in 2002 in all control sections was carried out practically equally, except of last section, where the pollution $\approx 1{,}9$ times is surpassed of the pollution of other sections. In 2003 the river is most of all polluted with marked parameter on initial and final sections. In 2002 the third section of the river is most of all polluted by parameter PO_4, and in 2003 namely this section is polluted less of all. The r. Choga runs in the r. Ochkhomuri in

this section. As we already have noted in 2002 the pollution of the r. Choga by parameter NO_3 ≈ 2 times are surpassed the pollution of 2003, and by parameter PO_4 - $\approx 1{,}32$ times. The pollution of the r. Ochkhomuri on the last section (where the r. Choga runs in it) in 2002 $\approx 2{,}7$ times are surpassed the pollution of 2003 by parameter NO_3 and $\approx 2{,}8$ times - by parameter PO_4. The mean annual volumes, computed by model and directly by measured meanings, brought in of polluting components by the river Ochkhomuri in the river Khobistsksli practically are equal among themselves. Brought by the river Ochkhomuri in the river Khobistsksli the mean annual meanings of polluting components on both considered components considerably has decreased after comparison with 2002: by parameter NO_3 from 7,119 ton/years till 3,685 ton/years (≈ 2 times), and by parameter PO_4 from 36,212 kg/years till 33,661 kg/years ($\approx 1{,}08$ times).

- The r. Chanistskali by parameters NO_3 and PO_4 both in 2002, and in 2003 is more polluted in the second section than in the first. In this section the river pollute not only by agricultural fields and cattle-breeding farms, but by waste water of the city Tsalendjikha too. The pollution of the river by parameter NO_3 in 2002 surpasses the pollution of 2003 and by parameter PO_4 the pollution of 2002 lags from the pollution of 2003. In particular, at 2002 the mean annual volume of the component NO_3 dropped by r. Chanistskali in the river Khobistskali is equal to 18,026 ton/year, which on the volume of 2003, 11,197 ton/year, surpass $\approx 1{,}6$ times, and mean annual volume of the component PO_4 in 2002 is equal to 88,515 kg / year, which lags from mean annual volume of 2003, 123,018 kg/years, $\approx 1{,}4$ times. Computed by mathematical models and directly by measured meanings brought by the river Chanistskali in the river Khobistskali volumes of polluting components coincide with each other by very high accuracy. In our opinion, one of the reasons of such good result consists that calculation of self purification coefficient of the river for considered components was possible for data of the river Chanistskali, which have taken advantage for other rivers too.
- The river Khobistskali in 2002 is most of all polluted in the first and in the last sections. On these sections, except of agricultural fields and cattle-breeding farms the river accordingly becomes polluted by waste water of the cities Chkhorotsku and Khobi. On the next place by pollution there is the fourth section of the river, where the river Chanistskali runs into it. In 2003 the river is almost equally polluted in the first and fourth sections, i.e. the sections on which work the city Chkhorotsku and the r. Chanistskali. The last section, where on the river work the city Khobi, is one of least polluted. This fact is very much interesting, which one more time confirms the reason that by the considered components the basic pollution sources of the rivers are agricultural fields and cattle -breeding farms. The pollution of the r. Khobistskali by the parameter NO_3 in 2002 surpasses the pollution of 2003 and by parameter PO_4 the pollution of 2002 lags behind pollution of 2003. In particular, by the river Khobistskali in the Black sea introduced the mean annual volume of the component NO_3 is equal to 62,772 ton/year, which surpasses the volume of 2003 43,605 ton/years $\approx 1{,}4$ times, and the mean annual volume of the component PO_4 for 2002 is equal 562,695 kg / year, which lag from the mean annual volume of 2003 673,473 kg/year $\approx 1{,}2$ times. The computed by the mathematical model and in direct by measured meanings brought by the river Khobistskali in the Black Sea volumes of

polluting components coincide with each other with acceptable accuracy, especially if we lake into account the above mentioned (in case of the river Choga).

Table 8.34. The computation results of pollutants mean annual meanings got from the appropriate sources in separate sections of the r. Choga during 2002, 2003

R. Choga					
Year	The pollutant ingredient	Until the first cross-section	Between the control section	Flow into the r. Ochkhomuri (by measuring)	Flow into the r. Ochkhomuri (by modeling)
2002	NO_3 kg/year	381.2	185.2	503.6	566.4
	PO_4 kg/year	1.68	2.5	3.8	4.18
2003	NO_3 kg/year	252.8	23.6	234.73	276.4
	PO_4 kg/year	2.2	0.972	2.814	3.172

Table 8.35. The computation results of pollutants mean annual meanings got from the appropriate sources in separate sections of the r. Ochkhomuri during 2002, 2003

R. Ochkhomuri							
Year	The pollutant ingredient	Until the first cross-section	The first section	The second section	The third section	Flow into the r. Khobistskali (by measu-ring)	Flow into the r. Kho-bistskali (by mode-ling)
2002	NO3 ton/year	1.494	1.392	1.459	2.774	7.390	7.119
	PO4 kg/year	9.170	8.316	15.663	3.063	36.375	36.212
2003	NO3 ton/year	1.125	0.8844	0.537	1.140	3.894	3.685
	PO4 kg/year	8.292	7.477	5.523	12.369	40.800	33.661

Table 8.36. The calculation results of pollutants mean annual meanings got from the appropriate sources in separate sites of the r. Chanistskali during 2002, 2003

R. Chanistskali					
Year	The pollu-tant ingre-dient	Until the first section	Between the control section	Flow into the r. Kho-bistskali (by measuring)	Flow into the r. Khobistskali (by modeling)
2002	NO3 ton/year	1.326	16.7	18.03	18.026
	PO4 kg/year	9.5	79.012	88.683	88.515
2003	NO3 ton/year	1.5	9.7	11.198	11.197
	PO4 kg/year	20.749	102.269	122.872	123.018

Table 8.37. The computation results of pollutants mean annual meanings got from the appropriate sources in separate sections of the r. Khobistskali during 2002, 2003

R. Khobistskali									
Year	The pollutant ingredient	Until the first section	In the first section	In the second section	In the third section	In the fourth section	In the fifth section	Flow into the black sea (by measuring)	Flow into the black sea (by mode-ling)
2002	NO3 ton/year	11.754	16.337	4.949	2.31	14.669	12.753	52.710	62.772
	PO4 kg/year	121.027	106.85	32.949	61.527	79.386	160.956	457.278	562.695
2003	NO3 ton/year	8.488	11.38	6.553	0.879	12.68	3.625	36.809	43.605
	PO4 kg/year	128.274	200.946	25.784	81.384	198.189	39.496	560.809	673.473

CONCLUSION

In the monograph from the single methodical point of view there are developed the mathematical models of diffusion of pollutants in the rivers and methods for marking decision. The problem of identification of emergency pollution sources in the rivers is formalized. The algorithms for the solution of stated problems are designed. Optimum and quasi-optimum algorithms of hypotheses testing are also developed. The one-, two- and three-dimensional mathematical models of pollutants transport and diffusion in the rivers are built under different initial and boundary conditions. The computation schemes of these models are optimized. The universal method of identification of nonlinear statistical models for the description of pollutants changes in the rivers is developed and the algorithms of its realization for the set of nonlinear functional dependences are given. The program packages of identification of excessive pollution sources and realization of mathematical models of

pollutants transport in the rivers are also developed. The designed methods and algorithms are incorporated into those packages, which are realized as the application software packages for IBM – compatible personal computers in accordance with generally accepted standards applicable to similar products through the world. They are loaded to the CD-ROM and are attached to this book. Users can exploit them as modern, convenient and reliable instruments at solution of the problems from the considered areas. Comprehensive experimental researches of designed software packages and algorithms realized in them have proved their high computing, operational and service qualities.

We believe the results given in this work are interesting and useful for a wide range of specialists and scientists working as in the field of applied mathematics, as in modeling and monitoring of pollution of natural waters, ecology, hydrology, power engineering, building of different structures on water objects etc. Their importance and practical value is the applied nature of the obtained theoretical results, which are submitted in the friendly form for comprehension and are ready (appended software packages) for direct application for the solution of practical tasks. Advantages of the elaborated methods and algorithms are shown not only through theoretical judgements and calculations, but also through the demonstration of results of particular calculus and modeling.

We believe the offered book will be of interest and useful not only for the experienced specialists and scientists, working in the relevant areas, but also for young, starting persons. It also will be useful for students and post-graduate students specializing in the respective areas.

Interested persons can obtain working copies of the developed packages for their practical use addressing to authors to the address: kartlos5@yahoo.com.

APPENDIX 1.
GENERATOR OF RANDOM VARIABLES OBEYING THE GIVEN PROBABILITY DISTRIBUTION LAWS

Modeling of random variables is made according to the following principle [1, 126, 191].

Let's assume that it is necessary to simulate random variable η with probability distribution density $\varphi(y)$. Let $\Phi(y)$ is its probability distribution function. Let ς be a uniformly distributed random variable with probability distribution density $f(x)$, $0 < x < 1$. Random variable η is determined from the following condition

$$\int_{-\infty}^{\eta} \varphi(y)\, dy = \varsigma ,$$

i.e. $\eta = \Phi^{-1}(\varsigma)$. Really

$$P(\eta < y) = P(\Phi^{-1}(\varsigma) < y) = P(\varsigma < \Phi(y)) = \Phi(y).$$

Standard uniformly distributed random variables are generated by means of standard procedure RANDOM.

APPENDIX 2.
GENERATOR OF NORMALLY DISTRIBUTED RANDOM VECTORS [212]

If m-dimensional random vector $\varsigma = (\varsigma_1,...,\varsigma_m)$, where $\varsigma_i \square N(\cdot;0,1)$, $i = 1,...,m$, and $\mathrm{cov}(\varsigma_i, \varsigma_j) = 0$ at $i \neq j$, is simulated and transformed according to expression

$$\eta = \gamma + \alpha \cdot K_1^{-1} \cdot \varsigma,$$

then $\eta = (\eta_1,...,\eta_m)$ will be normally distributed random vector with mathematical expectation γ and covariant matrix $W_{m\times m}$.

Matrices α, K_1 are defined in the paragraph 4.2.

APPENDIX 3.
GENERATOR OF MULTIDIMENSIONAL NORMAL MARKOVIAN SERIES WITH A GIVEN CONNECTIVITY DEPTH [1, 213]

Below is shortly described the results of the paragraph 3.7 which are used for direct generation of considered process.

A stationary Gaussian series is fully defined by giving the covariant matrix. Therefore, m-dimensional Gaussian Markovian series $X(t) = (x_1(t), x_2(t), ..., x_m(t))$, with connectivity depth N, may be represented in the following form:

$$x_p = \sum_{\ell=1}^{p-1} b_\ell^p x_\ell(t) + \sum_{i=1}^{m} \sum_{j=1}^{N} a_{ij}^p x_i(t-j) + \sigma_p \xi_p(t), \qquad \text{(A.3.1)}$$

where b_ℓ^p, a_{ij}^p are the coefficients that depend on auto- and inter-covariant functions of m-dimensional random series $X(t) = (x_1(t), x_2(t), ..., x_m(t))$; σ_p^2 is residual variance of random series $x_p(t)$; $\xi_p(t)$ is standard, normally distributed random variable.

The unknown coefficients and the residual variance in (A.3.1) are found by means of least-squares technique. With the following designations:

$$R'_{k,i}(|h-j|) = \begin{cases} R_{k,i}(|h-j|) & at \quad h \geq j, \\ R_{i,k}(|h-j|) & at \quad h < j, \end{cases}$$

$k, i = 1, ..., m; \quad j, n = 1, ..., N;$

$A_p^T = (b^p, a^p)_{1\times[m\cdot N+(p-1)]}; \quad C_p^T = (R_{k,i}(h))_{1\times m\cdot N};$

$B_p(R'_{k,i}(|h-j|)_{m\cdot N\times[m\cdot N+(p-1)]}, \quad p = 1, ..., m,$

where $R_{k,i}(|h-j|)$ are the corresponding covariances, the expression for the unknown coefficients assumes the following form:

$$A_p = B_p^+ \cdot C_p,$$

where B_p^+ is pseudoinverse matrix; expression for the residual variance is

$$\sigma_p^2 = R_p(0) - \sum_{\ell=1}^{p-1}\sum_{k=1}^{p-1} b_\ell^p b_k^p R_{\ell,k}(0) - \sum_{i=1}^{m}\sum_{j=1}^{N}\sum_{k=1}^{m}\sum_{\ell=1}^{N} a_{k\ell}^p a_{ij}^p R_{i,k}'(|\ell - j|) - 2\sum_{\ell=1}^{p-1}\sum_{j=1}^{N}\sum_{i=1}^{m} b_\ell^p a_{ij}^p R_{i,\ell}(j),$$

where $R_p(0)$ is variance of the p-th random process.

Let's introduce the following designations: γ_p required accuracy of Markovian series generation; Δ_R - maximum absolute error of calculation of covariant function one value.

If

$$\Delta_R \le \frac{\gamma_p}{N^{1/2}(\sum_{i=1}^{m}\beta_i^2)^{1/2}\|A_{p0}\|\{N^{1/2}[\sum_{i=1}^{m}(cond^+ B_i\|A_{i0}\|D_i)^2]^{1/2} + cond^+ B_p D_p\}};$$

$$D_i = \frac{[m^2N^2 + mN(i-1)]^{1/2}\|C_i\| + (mN)^{1/2}\|B_i\|}{\|B_i\|\cdot\|C_i\|}, i = 1,...,m,$$

holds for all $p = 1,...,m,$ the multidimensional Gaussian Markovian series is generated to the given accuracy with probability equal to or greater than $(1-\alpha)$. Here: $\|\cdot\|$ is Euclidean norm of the corresponding matrix; $cond^+ B_p = \|B_p\|\cdot\|B_p^+\|$ is conditionality number of matrix B_p; β_i is the value for which $P(|\hat{x}_i(t-j)| \le \beta_i) = 1-\alpha$ holds.

Sample size n, that ensures computation of covariant function values with absolute error not exceeding Δ_R, is determined from the following relation:

$$n = \max_{\{i\}}\{i + \frac{1}{\gamma_i\sqrt{\alpha}}[(n^*+1)R^2(0) + (n^*+1-i)R^2(i) + 2\cdot\sum_{j=1}^{n^*}(n^*+1-j)R^2(j) +$$

$$+2\cdot\sum_{j=1}^{n^*-i}(n^*+1-i-j)R(j+i)R(j-i)]^{1/2}\}, \quad i = 0,1,...,\max\{n,n^*\}.$$

Input information for this program is: $R_{i,k}(j)$, $i,k = 1,...,m$; $j = 1,...,N$; γ_p; Δ_R; α.

APPENDIX 4.
THE RESULTS OF REALIZATION OF DESCRIBED IN SECTION 3.2 GENERAL METHODOLOGY FOR IDENTIFICATION OF NONLINEAR REGRESSIONS FOR CERTAIN CLASS OF FUNCTIONAL DEPENDENCES AND PROPERTIES OF RESTORED DEPENDENCES

The considered set of functional dependences is defined on the basis of expert - estimations of leading experts of some institutes as most often meeting in researches.

1. GEOMETRICAL REGRESSION

The regression model is

$$y_i = a \cdot x_i^b + \varepsilon_i, \quad x_i > 0, \quad a > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

For definition of coefficients a and b the modified criterion of the least squares is used [1]:

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot \ln x_i - \ln y_i\right)^2 \Rightarrow \min_{\{a,b\}}, \qquad \text{(A.4.1)}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. By solving the optimization task (A.4.1) for unknown coefficients, we obtain

$$\begin{bmatrix} A \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & z_i \\ z_i & z_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} \ln y_i \\ z_i \cdot \ln y_i \end{bmatrix};$$

$z_i = \ln x_i$.

If σ_i^2 are unknown, it is possible to use their estimations

$$S_i^2 = \frac{1}{m_i} \cdot \sum_{k=1}^{m_i} y_{ik},$$

where y_{ik}, $k = 1,...,m_i$ - are repeated observations of y_i for given x_i.

2. EXPONENTIAL REGRESSION

The regression model is

$$y_i = a \cdot e^{bx_i} + \varepsilon_i, \quad x_i > 0, \quad a > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The modified criterion of the least squares has the following form

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot x_i - \ln y_i\right)^2 \Rightarrow \min_{\{a,b\}}, \tag{A.4.2}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Minimizing (A.4.2), we obtain

$$\begin{bmatrix} A \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & x_i \\ x_i & x_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \begin{bmatrix} 1 \\ x_i \end{bmatrix}.$$

3. LOGARITHMIC REGRESSION

The regression model is

$$y_i = a \cdot \ln(bx_i) + \varepsilon_i, \quad x_i > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\text{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The minimum of the weighing sum of discrepancies squares with weight factors $\lambda_i = 1/\sigma_i^2$ is achieved in a case, when the parameters a and b are determined by ratio: $b = e^{B/a}$;

$$\begin{bmatrix} B \\ a \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & z_i \\ z_i & z_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \cdot y_i \begin{bmatrix} 1 \\ z_i \end{bmatrix};$$

$$z_i = \ln x_i; \quad \lambda_i = 1/\sigma_i^2.$$

4. GEOMETRIC- EXPONENTIAL REGRESSION

The regression model is

$$y_i = a \cdot x_i^b \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\text{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The modified criterion of the least squares takes notes like this:

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot \ln x_i + c \cdot x_i - \ln y_i\right)^2 \Rightarrow \min , \qquad \text{(A.4.3)}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a.$. Minimum in (A.4.3) is obtained at

$$\begin{bmatrix} A \\ b \\ c \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & z_i & x_i \\ z_i & z_i^2 & x_i z_i \\ z_i & x_i z_i & x_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \begin{bmatrix} 1 \\ z_i \\ x_i \end{bmatrix};$$

$z_i = \ln x_i$; $\lambda_i = 1/\sigma_i^2$.

5. EXPONENTIAL REGRESSION WITH THE FREE MEMBER

The regression model is

$$y_i = a + b \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The criterion of the least squares has the following view:

$$S = \sum_{i=1}^{N} \lambda_i \cdot \left(a + b \cdot e^{cx_i} - \ln y_i\right)^2 \Rightarrow \min ,$$

where $\lambda_i = 1/\sigma_i^2$. The minimal value of quantity S at fixed value of c is obtained at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & E_i \\ E_i & E_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \cdot y_i \cdot \begin{bmatrix} 1 \\ E_i \end{bmatrix}$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - a\eta_1 - b\eta_2 .$$

The value of the parameter c, for which the function $S(c)$ is minimal, is determined by the iterative method of Hooke–Jeeves [4, 9]. Borders of search of the given parameter (hereinafter, where for minimization of the modified criterion of the least squares is used an iterative method) are determined by ratio (3.5), (3.6), i.e. by *modified method of trials* [73].

6. GEOMETRICAL REGRESSION WITH THE FREE MEMBER

The regression model is

$$y_i = a + b \cdot x_i^c + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

This task is equivalent to the restoration of dependence $a + b \cdot e^{cz}$ (considered in the previous Item) at the designation $z = \ln x$.

7. INVERSE EXPONENTIAL REGRESSION

The regression model is

$$y_i = a \cdot \left(1 - e^{-bx_i}\right) + \varepsilon_i,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of b is obtained at

$$a = \frac{\sum_{i=1}^{N} \lambda_i y_i \cdot \left(1 - e^{-bx_i}\right)}{\sum_{i=1}^{N} \lambda_i \cdot \left(1 - e^{-bx_i}\right)^2}$$

and is equal to

$$S(b) = \sum_{i=1}^{N} \lambda_i y_i \cdot \left(y_i - a \cdot \left(1 - e^{-bx_i}\right)\right).$$

The value of parameter b, for which the function $S(b)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of given parameter undertake similarly to borders for parameter c at restoration of dependence $f(a,b,c,x) = a + b \cdot e^{cx}$, (see point 5).

8. LINEAR – EXPONENTIAL REGRESSION

The regression model is

$$y_i = (a + bx_i) \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$, for fixed value of c, is obtained at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i E_i \cdot \begin{bmatrix} 1 & x_i \\ x_i & x_i^2 E_i \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i y_i E_i \cdot \begin{bmatrix} 1 \\ x_i \end{bmatrix};$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - a\eta_1 - b\eta_2 .$$

The value of the parameter c, for which the function $S(c)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of given parameter are determined by *the modified method of trials* (3.5), (3,6).

9. LINEAR – EXPONENTIAL DEPENDENCE WITH THE FREE MEMBER

The regression model is

$$y_i = h + (a + bx_i) \cdot e^{cx_i} + \varepsilon_i,$$

where h, a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$, for fixed value of c is obtained at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & E_i & x_i E_i \\ E_i & E_i^2 & x_i E_i^2 \\ x_i E_i & x_i E_i^2 & x_i^2 E_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i y_i \cdot \begin{bmatrix} 1 \\ E_i \\ x_i E_i \end{bmatrix};$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - h\eta_1 - a\eta_2 - b\eta_3 .$$

The value of the parameter c, for which the function $S(c)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (3.5), (3.6).

10. PRODUCT OF GEOMETRICAL DEPENDENCES

The regression model is

$$y_i = a \cdot x_i^c \cdot (1 - bx_i)^d + \varepsilon_i ,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The modified criterion of the least squares can be written down as follows

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + c \cdot \ln x_i + d \cdot (1 - bx_i) - \ln y_i\right)^2 \Rightarrow \min ,$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Minimal value of the variable S' at fixed value of b is obtained at

$$\begin{bmatrix} A \\ c \\ d \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = \ln x_i; \quad Q_i = \ln(1 - bx_i),$$

and is equal to

$$S'(b) = \sum_{i=1}^{N} \lambda_i' \cdot (\ln y_i)^2 - A\eta_1 - c\eta_2 - d\eta_3 .$$

The value of the parameter b, for which the function $S'(b)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (3.5), (3.6).

11. SUM OF EXPONENTIAL DEPENDENCES

The regression model is

$$y_i = a \cdot e^{cx_i} + b \cdot e^{dx_i} + \varepsilon_i ,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies $S(c,d)$ with weight factors $\lambda_i = 1/\sigma_i^2$, for fixed values of c and d is obtained at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} P_i^2 & P_i Q_i \\ P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i y_i \cdot \begin{bmatrix} P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{cx_i}; \quad Q_i = e^{dx_i},$$

and is equal to

$$S(c,d) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - a\eta_1 - b\eta_2 .$$

The values of the parameters c and d, for which the function $S(c,d)$ is minimal, are determined by an iterative method of Hooke–Jeeves. The borders of search of these parameters are determined by *the modified method of trials* (3.5), (3.6).

12. SUM OF GEOMETRICAL DEPENDENCES

The regression model is

$$y_i = a \cdot x_i^c + b \cdot x_i^d + \varepsilon_i,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The given task is equal to the restoration of the dependence $a \cdot e^{cz} + b \cdot e^{dz}$ (considered in previous Item) at the designation $z = \ln x$.

13. SUM OF EXPONENTIAL DEPENDENCES WITH THE FREE MEMBER

The regression model is

$$y_i = h + a \cdot e^{cx_i} + b \cdot e^{dx_i} + \varepsilon_i,$$

where h, a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies $S(c,d)$ with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed values of c and d is obtained at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix};$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \cdot y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{cx_i}; \quad Q_i = e^{dx_i},$$

and is equal to

$$S(c,d)=\sum_{i=1}^{N}\lambda_i\cdot y_i^2-h\eta_1-a\eta_2-b\eta_3.$$

The values of the parameters c and d, for which the function $S(c,d)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of these parameters are determined by *the modified method of trials* (3.5), (3.6).

14. SUM OF GEOMETRICAL DEPENDENCES WITH THE FREE MEMBER

The regression model is

$$y_i=h+a\cdot x_i^c+b\cdot x_i^d+\varepsilon_i,$$

where h, a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i=1,...,N$; $E(\varepsilon_i)=0$; $V(\varepsilon_i)=\sigma_i^2$; $\operatorname{cov}(\varepsilon_i,\varepsilon_k)=0$, $i\neq k$.

Considered task is equal to the restoration of the dependence $h+a\cdot e^{cz}+b\cdot e^{dz}$ (considered in previous Item) at the designation $z=\ln x$.

15. EXPONENTIAL – SINE WAVE REGRESSION

The regression model is

$$y_i=e^{cx_i}\cdot\left(a\cdot\cos(\omega x_i)+b\cdot\sin(\omega x_i)\right)+\varepsilon_i,$$

where a, b, c, ω are unknown coefficients determined by experimental data: x_i, y_i, $i=1,...,N$; $E(\varepsilon_i)=0$; $V(\varepsilon_i)=\sigma_i^2$; $\operatorname{cov}(\varepsilon_i,\varepsilon_k)=0$, $i\neq k$.

Minimal value of the weighed sum of squared discrepancies $S(c,\omega)$ with weight factors $\lambda_i=1/\sigma_i^2$, for fixed values of c and ω is obtained at

$$\begin{bmatrix}a\\b\end{bmatrix}=\xi^{-1}\cdot\begin{bmatrix}\eta_1\\\eta_2\end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} P_i^2 & P_i Q_i \\ P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i y_i \cdot \begin{bmatrix} P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{cx_i} \cdot \cos(\omega x_i); \quad Q_i = e^{cx_i} \cdot \sin(\omega x_i),$$

and is equal to

$$S(c,\omega) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - a\eta_1 - b\eta_2 .$$

The values of parameters c and ω, for which the function $S(c,\omega)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of these parameters are determined by *the modified method of trials* (3.5), (3.6).

At definition of the borders for the parameter ω, the fact that the difference among neighbouring zeros of the function $f(a,b,c,\omega,x)$ is equal to $\Delta x = \pi / \omega$ is also taken into account.

16. EXPONENTIAL – SINE WAVE REGRESSION WITH THE FREE MEMBER

The regression model is

$$y_i = h + e^{cx_i} \cdot (a \cdot \cos(\omega x_i) + b \cdot \sin(\omega x_i)) + \varepsilon_i ,$$

where h, a, b, c, ω are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimal value of the weighed sum of squared discrepancies $S(c,\omega)$ with weight factors $\lambda_i = 1/\sigma_i^2$, for fixed values of c and ω is obtained at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \cdot y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{cx_i} \cdot \cos(\omega x_i); \quad Q_i = e^{cx_i} \cdot \sin(\omega x_i),$$

and is equal to

$$S(c,\omega) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - h\eta_1 - a\eta_2 - b\eta_3.$$

The values of parameters c and ω, for which the function $S(c,\omega)$ is minimal, is determined by an iterative method of Hooke–Jeeves. The borders of search of these parameters are determined by *the modified method of trials* (3.5), (3.6).

At definition of borders for parameter ω, the fact that the difference among neighbouring points of a maximum (and points of a minimum) of the function $f(h,a,b,c,\omega,x)$ is equal to $\Delta x = \pi/\omega$ is also taken into account.

17. POLYNOMIAL REGRESSION

The regression model is

$$y_i = \sum_{k=0}^{m} p_k x_i^k + \varepsilon_i,$$

where $p_0,...,p_m$ are unknown coefficients determined by experimental data: x_i, y_i, $i = 1,...,N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\mathrm{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

Minimum of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$ is obtained at

$$\begin{bmatrix} p_0 \\ p_1 \\ \dots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is matrix of the size $M \times M$ with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot x_L^{j+k-2};$$
$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot y_L x_L^{k-1};$$
$$\lambda_L = 1/\sigma_L^2.$$

In the program is realized the possibility of an automatic choice of the model's power, i.e. identification not only the coefficients, but also a power of the polyinomial by the following algorithm.

Let minimal variance corresponds to the model of power m_0; $1 \le m_0 \le n$, where n is possible greatest power of the model. Let's designate this variance by $S^2(m_0)$. Let's construct a confidence interval

$$\frac{(N - m_0 - 1) \cdot S^2(m_0)}{\chi_{1-\alpha/2}} \le \sigma^2(m_0) \le \frac{(N - m_0 - 1) \cdot S^2(m_0)}{\chi_{\alpha/2}},$$

where $\sigma^2(m_0)$ is unknown true value of the variance; $\chi_{\alpha/2}$ and $\chi_{1-\alpha/2}$ are the quantiles of the orders $\alpha/2$ and $1-\alpha/2$, respectively, of the χ^2 distribution law with $N - m_0 - 1$ degree of freedom; $1-\alpha$ is the confidence probability.

As a restored dependence we shall accept the model with the minimal power from the set of identified models, the variances of which falled in the constructed confidentce interval.

The choice of model's power is similarly carried out at identification of other dependences for which it is necessary.

18. GEOMETRICAL – POLYNOMIAL REGRESSION

The regression model is

$$y_i = x_i^c \cdot \sum_{k=0}^{m} p_k x_i^k + \varepsilon_i,$$

where $c, p_0,...,p_m$ are unknown coefficients determined by experimental data: x_i, y_i, $i=1,...,N$; $E(\varepsilon_i)=0$; $V(\varepsilon_i)=\sigma_i^2$; $\text{cov}(\varepsilon_i,\varepsilon_k)=0$, $i\neq k$.

Minimal value of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of c, we obtain for

$$\begin{bmatrix} p_0 \\ p_1 \\ \dots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_M \end{bmatrix},$$

where $M = m+1$; ξ is the matrix of the size $M \times M$ with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot x_L^{j+k+2c-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot y_L x_L^{k+c-1},$$

and is equal to

$$S(c) = \sum_{L=1}^{N} \lambda_L \cdot y_L^2 - \sum_{k=1}^{M} p_{k-1}\eta_k .$$

The value of the parameter c, for which the function $S(c)$ is minimal, is determined by the iterative method of Hooke–Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (3.5), (3.6).

19. EXPONENTIAL – POLYNOMIAL REGRESSION

The regression model has the following form

$$y_i = e^{cx_i} \cdot \sum_{k=0}^{m} p_k x_i^k + \varepsilon_i,$$

where $c, p_0,...,p_m$ are unknown coefficients determined by experimental data: x_i, y_i, $i=1,...,N$; $E(\varepsilon_i)=0$; $V(\varepsilon_i)=\sigma_i^2$; $\text{cov}(\varepsilon_i,\varepsilon_k)=0$, $i\neq k$.

Minimal value of the weighed sum of squared discrepancies with weight factors $\lambda_i = 1/\sigma_i^2$, for fixed value of c, we obtain for

$$\begin{bmatrix} p_0 \\ p_1 \\ \dots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is the matrix of the size $M \times M$ with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot \exp(2cx_L) \cdot x_L^{j+k-2};$$
$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot \exp(2cx_L) \cdot y_L x_L^{k-1},$$

and is equal to

$$S(c) = \sum_{L=1}^{N} \lambda_L \cdot y_L^2 - \sum_{k=1}^{M} p_{k-1}\eta_k .$$

The value of the parameter c, for which the function $S(c)$ is minimal, is determined by the iterative method of Hooke–Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (3.5), (3.6).

20. LOGARITHMIC – POLYNOMIAL REGRESSION

The regression model has the following form

$$y_i = c \cdot \ln\left(\sum_{k=0}^{m} p_k x_i^k\right) + \varepsilon_i,$$

where $c, p_0, ..., p_m$ are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$.

The modified criterion of the least squares has the following form

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(\sum_{k=0}^{m} p_k x_i^k - \exp(y_i / c) \right)^2 \Rightarrow \min ,$$

where $\lambda_i' = \lambda_i \cdot \exp(-2y_i / c)$. Minimal value of the variable S', for fixed value of c, we obtain for

$$\begin{bmatrix} p_0 \\ p_1 \\ \dots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is the matrix of the size $M \times M$ with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L' \cdot x_L^{j+k-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L' \cdot \exp(y_L / c) \cdot x_L^{k-1},$$

and is equal to

$$S(c) = \sum_{L=1}^{N} \lambda_L' \cdot \exp(2y_L / c) - \sum_{k=1}^{M} p_{k-1} \eta_k .$$

The value of the parameter c, for which the function $S'(c)$ is minimal, is determined by the iterative method of Hooke–Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (3.5), (3.6).

21. PERIODIC REGRESSION

Let us consider model

$$y_j = f(t_j) + \varepsilon_j, \quad j = 1,...,N,$$

where $E(\varepsilon_i) = 0$; $V(\varepsilon_i) = \sigma_i^2$; $\operatorname{cov}(\varepsilon_i, \varepsilon_k) = 0$, $i \neq k$; $f(t)$ is a periodic function with the period $T = 2\pi / \omega$ [1,104].

The consecutive values t_j of the independent variable should be equidistanced from each other with the step T/r, where r - *the number of the measured values in a period* – is integer, greater than or equal to 3; the general number of measured values N should be greater than or equal to $2r$; moreover, the number N should be divided by r without a remainder. If the latest condition is broken, then for dermition of the unknown parameters are only considered the first rp values of t_j and y_j, and other values are not taken into account; here p is integer component of the number N/r.

The considered dependence satisfies the condition $f(t_{j+r}) = f(t_j)$. Hence, the following representation is possible

$$f(t_j) = A_0 + \sum_{k=1}^{(r-1)/2} \left(A_k \cdot \cos(2\pi kj/r) + B_k \cdot \sin(2\pi kj/r) \right),$$

if r is odd number and

$$f(t_j) = A_0 + \sum_{k=1}^{r/2-1} \left(A_k \cdot \cos(2\pi kj/r) + B_k \cdot \sin(2\pi kj/r) \right) + A_{r/2} \cdot (-1)^j,$$

if r is even number.

Thus, the restored dependence looks like

$$f(A_0,...,A_{m+1},B_1,...,B_m,t) = A_0 + \sum_{k=1}^{m+1} A_k \cdot \cos(k\omega t) + \sum_{k=1}^{m} B_k \cdot \sin(k\omega t),$$

where m is integer component of the number $(r-1)/2$; $A_0,...,A_{m+1}$, $B_1,...,B_m$ are the parameters of approximation, and, in case of odd r, $A_{m+1} = 0$, and, in case of even r, $A_{m+1} = A_{r/2}$.

The estimations by the method of least squares of the parameters of approximation are calculated so:

$$\hat{A}_0 = \frac{1}{N} \cdot \sum_{j=1}^{N} y_j \ ;$$

$$\hat{A}_k = \frac{2}{N} \cdot \sum_{j=1}^{N} y_j \cdot \cos(2\pi kj/r); \ \ \hat{B}_k = \frac{2}{N} \cdot \sum_{j=1}^{N} y_j \cdot \sin(2\pi kj/r), \ (k = 1,...,m)$$

and

$$\hat{A}_{r/2} = \frac{1}{N} \cdot \sum_{j=1}^{N} y_j \cdot (-1)^j$$

at even r.

Variances of A_0 and $A_{r/2}$ are equal to σ^2 / N, and variances of A_k and B_k are equal to $2\sigma^2 / N$ $(k = 1,..., m)$. The unbiased estimation of the variance σ^2 is calculated by the formula

$$S^2 = \frac{1}{N-r} \cdot \left(\sum_{j=1}^{N} y_j^2 - N \cdot \left(A_0^2 + A_{m+1}^2 \right) - \frac{1}{2} \cdot \sum_{k=1}^{m} \left(A_k^2 + B_k^2 \right) \right)^2 . \qquad \text{(A.4.4)}$$

After calculation of the coefficients A_k and B_k, for every $k = 1,..., m$, is tested zero hypothesis $H_0 : A_k = \mathrm{B_k} = 0$. If this hypothesis is true then the statistics

$$v^2 = \frac{N \cdot R^2(k)}{4S^2},$$

where $R^2(k) = A_k^2 + B_k^2$, and S^2 is calculated by (A.4.4), is distributed by the Fisher's F distribution law with 2 and $N - r$ degrees of freedom. Thus, zero hypothesis is accepted if

$$v^2 \le v_{1-\alpha}^2 (2, N - r),$$

where α is the given significance level, $v_{1-\alpha}^2 (2, N - r)$ is the quantile of $1 - \alpha$ order of the Fisher distribution with $(2, N - r)$ degrees of freedom.

Automatic choosing the model's order is realized similarly to Item 17.

22. REGRESSION ANALYSIS

At identification of the above-stated functional dependences, in developed by authors of this book software package SDpro is an opportunity of switching on of the mode of operation for testing of regression model on the adequacy [93, 94, 101, 226]. In this mode of operation, the hypothesis about conformity of restored dependence to experimental data is tested by the following algorithm. The interval of representation of independent variable $(x_{\min}, x_{\max})$ is divided into K groups and there is calculated

$$v^2 = \frac{\frac{1}{K-m}\cdot\sum_{i=1}^{K} m_i\left|\bar{y}_i - f\left(\hat{a}, x_i^0\right)\right|^2}{\frac{1}{N-K}\cdot\sum_{i=1}^{K}\sum_{k=1}^{m_i}\left|y_{ik} - \bar{y}_i\right|^2},$$

where N is the size of sample; m is the number of estimated parameters of the restored functional dependence $f(a,x)$; m_i is the number of the measurements which fall into i th interval; x_i^0 is an average point of i th interval of groupping of data; $\bar{y}_i$ -is the arithmetic mean of the dependent variable falled into i th interval; $f\left(\hat{a}, x_i^0\right)$ is the value of the restored regression in the point x_i^0, $\hat{a}$ are the estimations of unknown parameters; y_{ik} is k th by the order value of the dependent variable falled into i th interval.

If there takes place

$$v_{\alpha/2}^2 < v^2 < v_{1-\alpha/2}^2,$$

where $v_{\alpha/2}$ and $v_{1-\alpha/2}$ are the quantiles of the orders $\alpha/2$ and $1-\alpha/2$, respectively, of the Fisher's distribution with $(K-m, N-K)$ degrees of freedom, then there is made decision that the restored regression does not contradict to the experimental data with probability $1-\alpha$. Here $1-\alpha$ is confidence probability.

If $v^2 < v_{\alpha/2}^2$ then on the display is brought out the message "simplify regression", i.e. for restoration of functional dependence it is necessary to choose more simple dependence among offered in the menu. If $v^2 > v_{1-\alpha/2}^2$ then on the display is brought out the message "complicate regress" and we choose more complex regression dependence among offered in the menu.

In the program of realization of this algorithm is an opportunity to set any allowable value of K - number of groups (interval of allowable values is indicated in the bottom line of the display) and α - the significance level of criterion.

23. MULTIPLE LINEAR REGRESSION

In the present task, in contradistinction to all the tasks considered above, a dependent variable is represented as a function of m independent variables $X_1,...,X_m$. The regression model looks like [105]

$$y_i = \sum_{k=1}^{m} A_k X_{ki} + \varepsilon_i,$$

where it is necessary to determine unknown coefficients $A_1,...,A_m$ on the basis of experimental data: y_i, x_{ki}, $k=1,...,m$, $i=1,...,N$; $E(\varepsilon_i)=0$; $V(\varepsilon_i)=\sigma_i^2$; $\mathrm{cov}(\varepsilon_i,\varepsilon_k)=0$, $i\neq k$.

The criterion of the least squares can be written down as:

$$S=\sum_{i=1}^{N}\lambda_i\cdot\left(\sum_{k=1}^{m}A_kX_{ki}-y_i\right)^2\Rightarrow\min,$$

where $\lambda_i=1/\sigma_i^2$. The minimum is obtained for

$$\begin{bmatrix}A_1\\A_2\\...\\A_m\end{bmatrix}=\xi^{-1}\cdot\begin{bmatrix}\eta_1\\\eta_2\\...\\\eta_m\end{bmatrix},$$

where ξ is the matrix of the size $m\times m$ with elements

$$\xi_{jk}=\sum_{L=1}^{N}\lambda_L\cdot X_{jL}X_{kL};$$

$$\eta_k=\sum_{L=1}^{N}\lambda_L\cdot y_LX_{kL}\ .$$

24. THE BASIC PROPERTIES OF RESTORED DEPENDENCES

Geometrical Dependence

$$f(x)=a\cdot x^b\ .$$

The graphs of the function $f(x)$ are given in Figure A.4.1 a) and b) at $a>0$ and different, accordingly, positive and negative values of the parameter b. At $a<0$, the appropriate graphs can be obtained from the presented in Figure A.4.1 by looking-glass reflection concerning the axis x. At $b<0$, the axes of coordinates serve as asymptotes of the graphs.

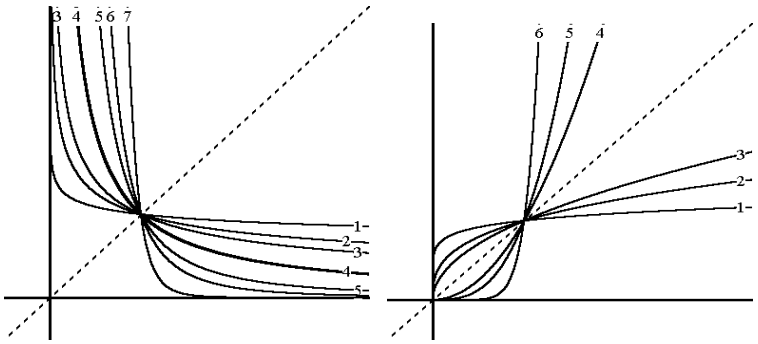


Figure A.4.1. The graph of the function $y = x^b$ at different meanings of b:

a) (positive values of b)
b = 1/8(1),b = 2(4),
b = 1/3(2),b = 3(5),
b = 1/2(3),b = 8(6).

b) (negative values of b)
b = –1/8(1),b = –2 (5),
b = –1/3(2),b = –3 (6),
b = –1/2(3),b = –8 (7).
b = –1 (4).

Exponential Dependence

$$f(x) = a \cdot e^{bx}.$$

The graphs of the function $f(x)$ are given in Figure A.4.2 at $a = 1$ and different values of the parameter b. The graphs pass through the point {0,1} and have the common asymptote, coinciding with the axis x.

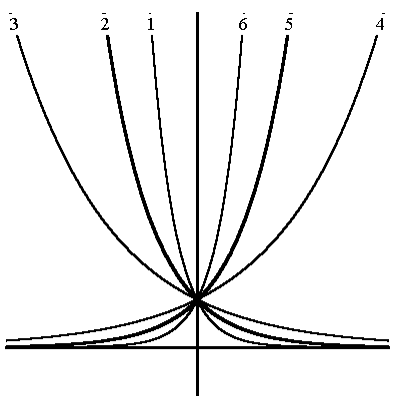


Figure A.4.2. The graph of the function $y = e^{bx}$ at different values of b:

a = –2 (1), a = 1/2 (4),
a = –1 (2), a = 1 (5),
a = –1/2(3), a = 2 (6).

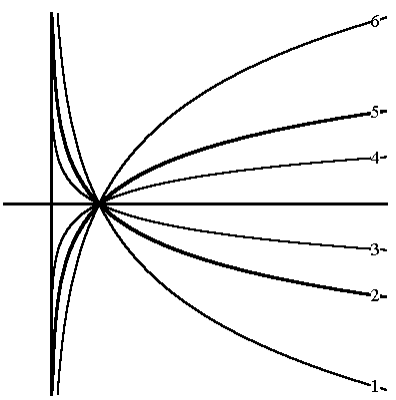


Figure A.4.3. The graph of the function $y = a \cdot \ln x$ at different values of a:

b = –2 (1), b = 1/2 (4),
b = –1 (2), b = 1 (5),
b = –1/2(3), b = 2 (6).

Logarithmic Dependence

$$f(x) = a \cdot \ln(bx).$$

The graphs of the function $f(x)$ are given in Figure A.4.3 at $b = 1$ and different values of the parameter a. The graphs pass through the point {1,0} and have common asymptote, coinciding with the axis y. At $b \neq 1$ the graphs of the function $f(x)$ can be obtained from the presented in Figure A.4.3 by shifting the latest one along the axis of ordinates on the distance $a \cdot \ln b$.

Geometric-exponential Dependence

$$f(x) = a \cdot x^b \cdot e^{cx}, \text{ at } x > 0.$$

If the number $x_0 = -b/c$ belongs to the domain of definition of the function $f(x)$ (i.e. if $bc < 0$), then the considered function has unique extreme point in $x = x_0$, otherwise it has not extreme points. If the graph of the present function has a point of inflection, then the abscess of this point is equal to

$$x_1 = \frac{-b + \sqrt{b}}{c} \text{ or } x_2 = \frac{-b - \sqrt{b}}{c}.$$

The graphs of the function $f(x)$ are submitted in Figure A.4.4 at $a > 0$; at $a < 0$ the appropriate graphs can be obtained from the presented in Figure A.4.4 by looking-glass reflection concerning the axis x. Depending on the values of the parameters b and c, eight cases are possible:

a) at $c > 0$ and $b > 1$, the function increases monotonically; the graph touchs the axis x in the point {0,0};
b) at $c > 0$ and $b = 1$ the function increases monotonically; the graph passes through the point {0,0} and touchs the straight line $y = x$ in this point;
c) at $c > 0$ and $0 < b < 1$ the function increases monotonically; the graph touchs the axis y in the point {0,0} and has a point of inflection with the abscess x_1;
d) at $c > 0$ and $b < 0$ the function has a minimum in the point x_0; the axis y is the asymptote of the graph;
e) at $c < 0$ and $b > 1$ the function has a maximum in the point x_0; the graph touchs the axis x in the point {0,0} and has two points of inflection; the axis x is the asymptote;

f) at $c<0$ and $b=1$ the function has a maximum in the point $x_0=-1/c$; the graph passes through the point $\{0,0\}$ and touchs the straight line $y=ax$ in this point; has one point of inflection with the abscess $x_2=-2/c$;

g) at $c<0$ and $0<b<1$ the function has a maximum in the point x_0; the graph touchs the axis y in the point $\{0,0\}$ and has one point of inflection with the abscess x_2;

h) at $c<0$ and $b<0$ the function decreases monotonically; the axes of ordinates are the asymptotes of the graph.

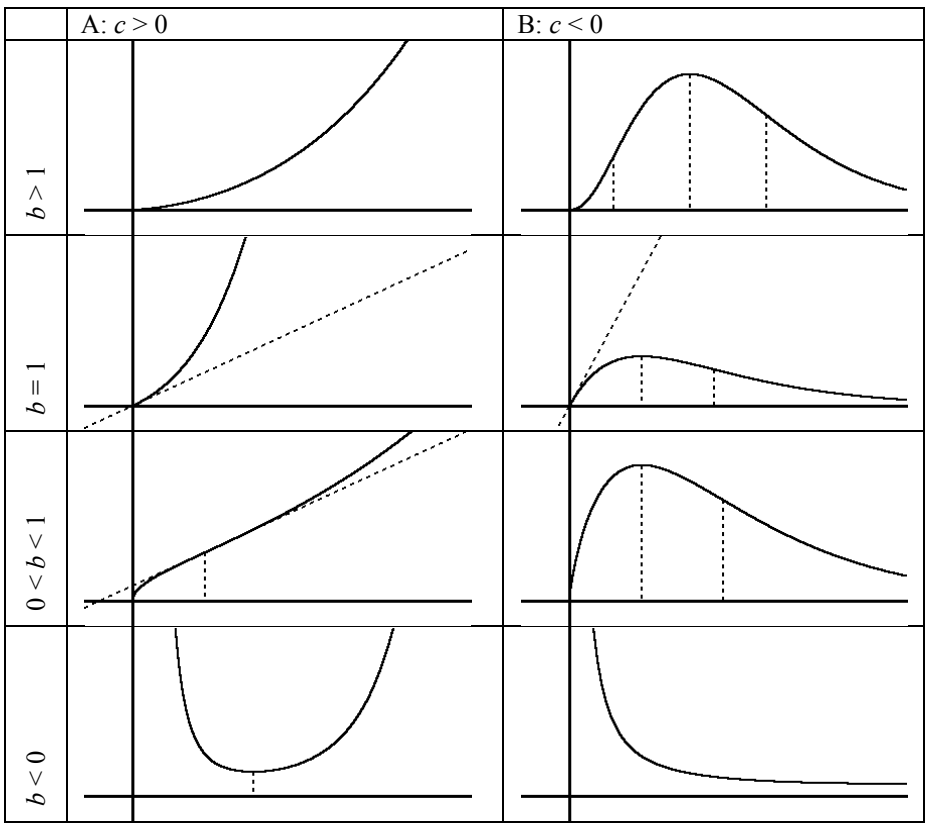


Figure A.4.4. The graph of the function $y = a \cdot x^b \cdot e^{cx}$ at $a > 0$ and different ranges of values of the parameters b and c.

Inverse-exponential Dependence

$$f(x)=a\cdot\left(1-e^{-bx}\right).$$

The graphs of function $f(x)$ are presented in Figure A.4.5 at $a>0$ and different positive values of the parameter b. The graphs pass through starting point of the co-ordinates

and have common horizontal asymptote, set by the equation $y = a$. At $a < 0$, the appropriate graphs can be obtained from presented in Figure A.4.5 by looking-glass reflection concerning the axis x.

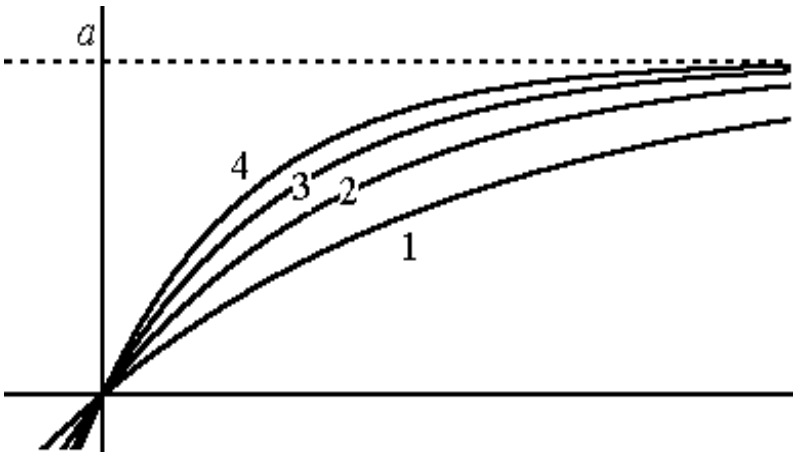


Figure A.4.5. The graph of the function $y = a \cdot (1 - e^{-bx})$ at different values of b: $b = 0.5$ (1); $b = 0.75$ (2); $b = 1$ (3); $b = 1.25$ (4).

Geometrical Dependence with the Free Member

$$f(x) = a + b \cdot x^c .$$

The graphs of the presented function can be obtained from the considered above graphs of geometrical dependence $f(x) = b \cdot x^c$ by shifting the latest one along the axis of ordinate on the distance a.

Exponential Dependence with the Free Member

$$f(x) = a + b \cdot e^{cx} .$$

The graphs of this function can be obtained from the considered above graphs of exponential dependence $f(x) = b \cdot e^{cx}$ by shifting the latest one along the axis of ordinate on the distance a.

Linear-Exponential Dependence

$f(x) = (a + bx) \cdot e^{cx}$ at $bc \neq 0$.

This function has a unique point of extreme

$$x_0 = -1/c - a/b,$$

being the point of minimum at $b > 0$ and point of maximum at $b < 0$.

The graph of this function has a unique point of inflection with the abscess

$$x_{\text{inf}} = -2/c - a/b.$$

The function $f(x)$ become equal to zero at $x = x_z = -a/b$.

At $x \to -\infty \cdot signc \quad f(x) \to 0$; at $x \to +\infty \cdot sign\ c \quad f(x) \to +\infty \cdot sign(bc)$.

Here

$$signx = \begin{cases} -1 \quad at \quad x < 0, \\ 1 \quad at \quad x > 0. \end{cases}$$

The graphs of the dependence $f(x)$ from $x + a/b$ are presented in Figure A.4.6 at different signs of b and c.

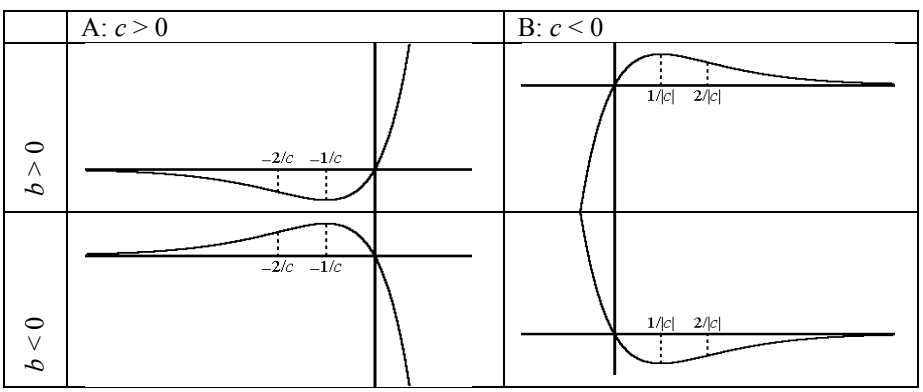


Figure A.4.6. The graph of the dependence $y = (a + b\,x)\cdot e^{cx}$ from $t = x + a/b$ at different signs of the parameters b and c.

Linear-exponential Dependence with the Free Member

$$f(x) = h + (a + bx) \cdot e^{cx}.$$

The graphs of this function can be obtained from the considered above graphs of the linear-exponential dependences

$$f(x) = (a + bx) \cdot e^{cx}$$

by shifting the latest one along the axis of ordinates on the distance h.

Product of Geometrical Dependences

$$f(x) = a \cdot x^c \cdot (1 - bx)^d .$$

The conditions are assumed executed: $a, b, c, d \neq 0;\ 0 < x < 1/b$ at $b > 0$ or $0 < x < +\infty$ at $b < 0$. Let us designate

$$x_0 = \frac{c}{b \cdot (c + d)};$$

then $1 - bx_0 = d/(c + d)$.

If the number x_0 belongs to the domain of definition of the function $f(x)$, then the considered function has unique extremum in the point $x = x_0$; otherwise it has not extremums. If the graph of this function has a point of inflection, then the abscess of this point is equal to x_1 or x_2, where bx_1 and bx_2 are the roots of the quadratic equation

$$(c + d)((c + d - 1) \cdot x^2 - 2c \cdot (c + d - 1) \cdot x + c \cdot (c - 1) = 0 .$$

The graphs of the function $f(x)$ are presented in Figure A.4.7 at $a > 0$; at $a < 0$, the appropriate graphs can be obtained from given in Figure A.4.7 by looking-glass reflection concerning concerning the axis x. Depending on the signs of the parameters b, c and d, the different cases are possible.

a) $b > 0, c > 0$ and $d > 0$. The function $f(x)$ has a maximum in the point x_0; at $x \to 0$ and at $x \to 1/b$ $f(x) \to 0$;

b) $b > 0, c > 0$ and $d < 0$. The function increases everywhere; at $x \to 0$ $f(x) \to 0$; at $x \to 1/b$, $f(x) \to +\infty$; the straight line $x \to 1/b$ is the asymptote of the graph of the considered function.

c) $b > 0, c < 0$ and $d > 0$. The function decreases everywhere; at $x \to 0$ $f(x) \to +\infty$; at $x \to 1/b$, $f(x) \to 0$; the axis y is the asymptote of the graph of the considered function.

d) $b > 0, c < 0$ and $d < 0$. The function has a minimum in the point x_0; at $x \to 0$ and at $x \to 1/b$, $f(x) \to +\infty$; the graph of the function has two vertical asymptote: $x = 0$ and $x = 1/b$.

e) $b < 0, c > 0$ and $c + d > 0$. The function increases monotonically; at $x \to 0$ $f(x) \to 0$; at $x \to +\infty$ $f(x) \to +\infty$.

f) $b < 0, c > 0$ and $c + d < 0$. The function has a maximum in the point x_0; at $x \to 0$ and at $x \to +\infty$, $f(x) \to 0$.

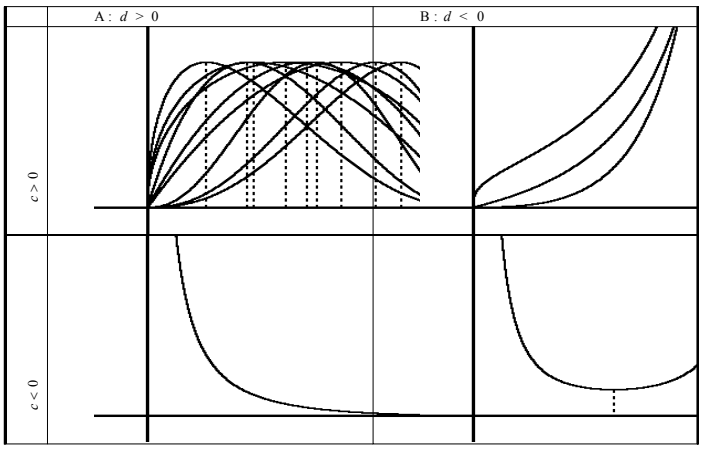
g) $b < 0, c < 0$ and $c + d > 0$. The function has a minimum in the point x_0; at $x \to 0$ and at $x \to +\infty$, $f(x) \to 0$.

h) $b < 0, c < 0$ and $c + d < 0$. The function decreases monotonically; at $x \to 0$ $f(x) \to +\infty$; at $x \to +\infty$, $f(x) \to 0$; the axes of ordinates are the asymptotes of the graph of the considered function.

i) At $x \to 0$, $f(x) \sim a \cdot x^c$. From here follows that at $c > 0$ and any a, b, d the graph of the function $f(x)$, in the point $\{0,0\}$, concerns either to the axis of abscess (at $c > 1$), or to straight line $y = ax$ (at $c = 1$), or to axis of ordinates (at $0 < c < 1$). At $b < 0$ the graphs of the function $f(x)$ behave similarly to the appropriate graphs of the function $\varphi(x) = a \cdot x^c \cdot e^{(c+d)x}$ (see Figure A.4.4).

j) At $b > 0, d > 0$ and any a and c, the graph of the function $f(x)$, in the point $\{0, 1/b\}$, concerns either to the axis of abscess (at $d > 1$), or to straight line $y = ab^{-c} - adb^{1-c} \cdot x$ (at $d = 1$), or to axis of ordinates (at $0 < d < 1$).

I: $b > 0$



II: $b < 0$

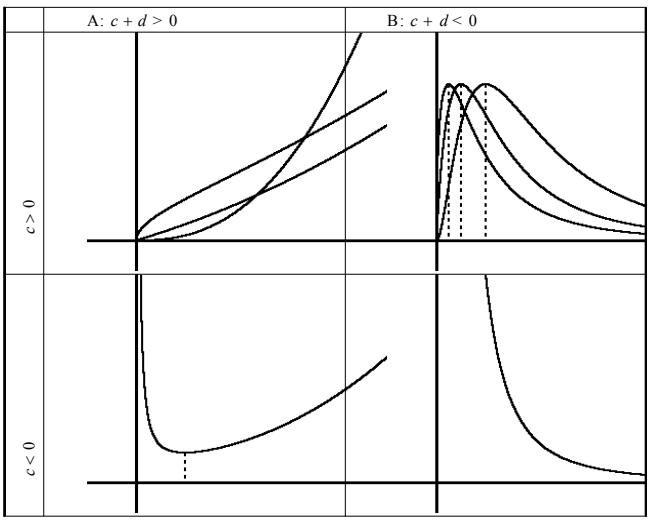


Figure A.4.7. The graph of the function $y = a \cdot x^c \cdot (1 - b\,x)^d$ at $a > 0$ and different regions of change of the parameters b, c, d.

The Sum of Exponential Dependences

$$f(x) = a \cdot e^{cx} + b \cdot e^{dx}.$$

Let $c < d$. Then

a) at $abcd < 0$, the point

$$x_0 = (d - c)^{-1} \cdot \ln\left(-\frac{ac}{bd}\right)$$

is a unique point of extremum of the function $f(x)$, otherwise the considered function has not the extremums;

b) at $ac > 0$ and $bd > 0$, the function $f(x)$ increases everywhere;

c) at $ac < 0$ and $bd < 0$, the function $f(x)$ decreases everywhere;

d) at $ac > 0$ and $bd < 0$, the function $f(x)$ has a maximum at $x = x_0$;

e) at $ac < 0$ and $bd > 0$, the function $f(x)$ has a minimum at $x = x_0$;

f) at $ab < 0$, the point

$$x_{\text{inf}} = (d-c)^{-1} \cdot \ln\left(-\frac{ac^2}{bd^2}\right)$$

g) is a unique point of inflection of the graph of the function $f(x)$, otherwise the graph of the considered function has not the points of inflection.

The graphs of the function $f(x)$ at $|c| < |d|$ and different signs of the parameters a, b, c, d are presented in Figure A.4.8.

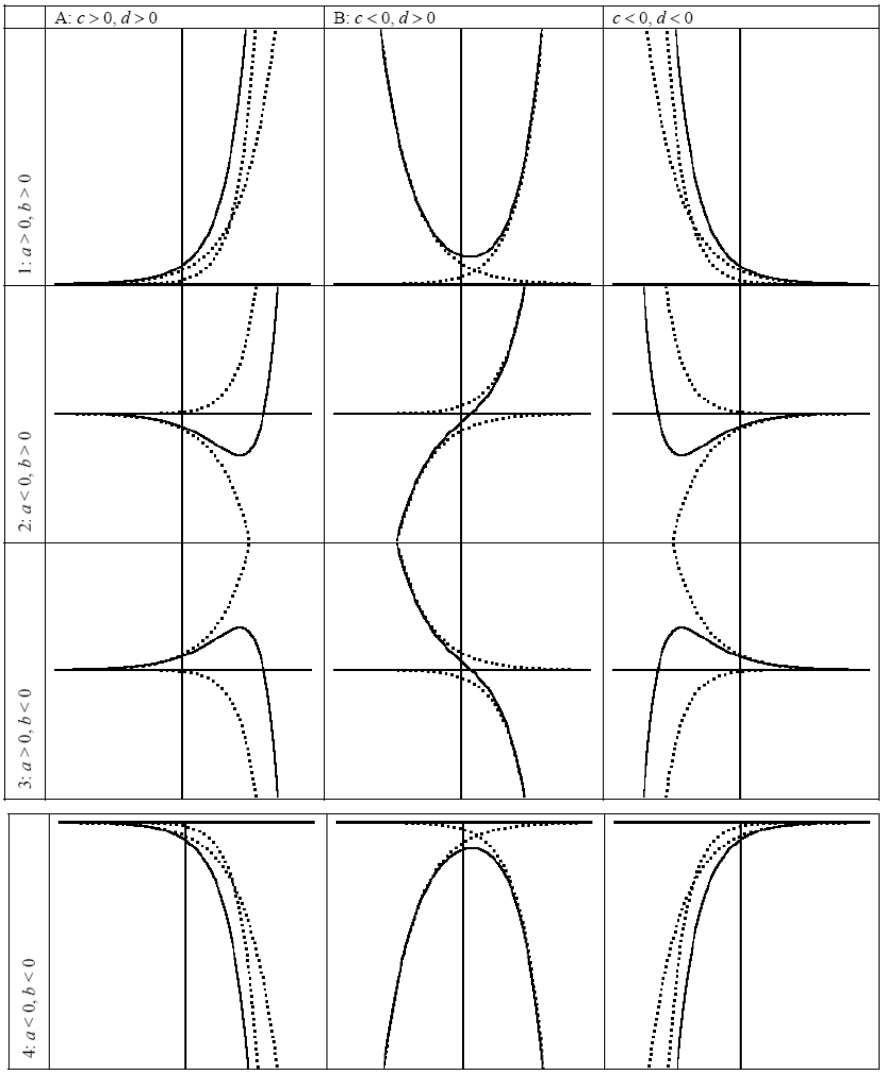


Figure A.4.8. The graph of the function $y = a \cdot e^{cx} + b \cdot e^{dx}$ at different signs of the parameters a, b, c, d.

Depending on the signs of the parameters a, b, c, d, it is possible to choose the following four types.

a) $ab > 0$ and $cd > 0$ (the squares A-1, C-1, A-4, C-4 in Figure A.4.8): the function is monotonicall everywhere; there are not extremums and zeros; the graph has not points of inflection; the axis x is the asymptote.

b) $ab > 0$ and $cd < 0$ (the squares B-1 and B-4 in Figure A.4.8): the function has one extremum (minimum at $a > 0$ and maximum at $a < 0$); it has not zeros; the graph has not points of inflection and the asymptotes;

c) $ab < 0$ and $cd > 0$ (the squares A-2, C-2, A-3, C-3 in Figure A.4.8): the function has one extremum (maximum at $a \cdot (d - c) > 0$ and minimum at $a \cdot (d - c) < 0$) and one zero; the graph has one point of inflection; the axis x is the asymptote;

d) $ab < 0$ and $cd < 0$ (the squares B-2 and B-3 in Figure A.4.8): the function has not extremums, it is monotonicall everywhere; it has one zero; the graph has one point of inflection; it has not the asymptotes.

The Sum of Geometrical Dependences

$$f(x) = a \cdot x^c + b \cdot x^d .$$

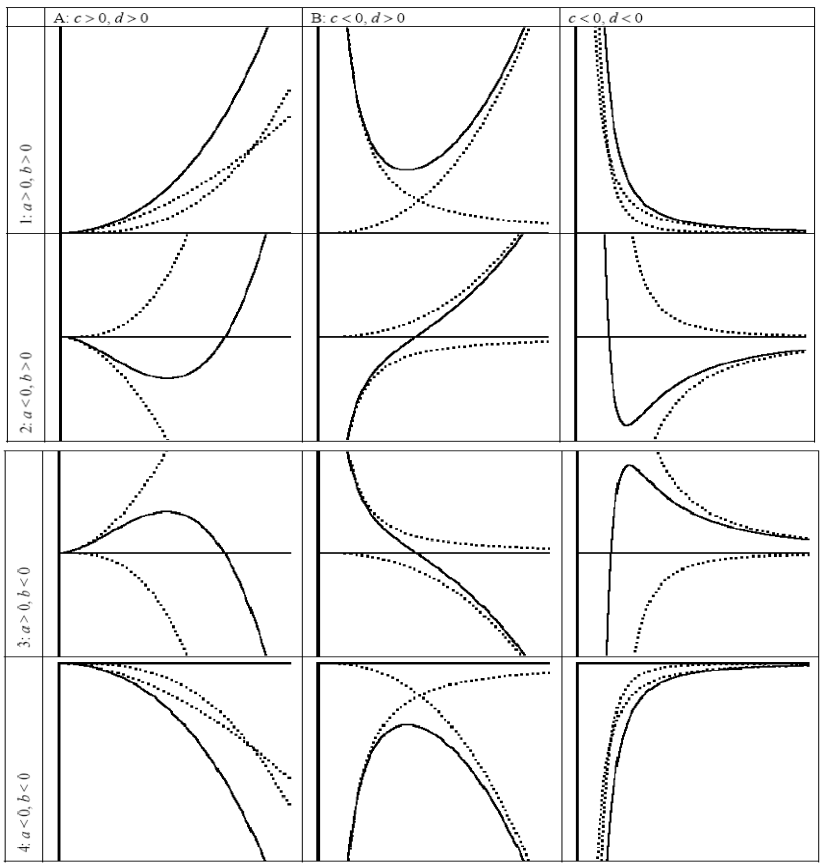


Figure A.4.9. The graph of the function $y = a \cdot x^c + b \cdot x^d$ at different signs of the parameters a, b, c, d.

The function $f(x)$ will be transformed to the considered above function

$$F(x) = a \cdot e^{ct} + b \cdot e^{dt}$$

at replacement of the independent variable $t = \ln x$. In Figure A.4.9 are presented the graphs of the function $f(x)$ at $|c| < |d|$ and different signs of the parameters a, b, c, d .

The Sum of Exponential Dependences with the Free Member

$$f(x) = h + a \cdot e^{cx} + b \cdot e^{dx}.$$

The graphs of this function can be obtained from the considered above graphs of the sum of exponential dependences

$$F(x) = a \cdot e^{cx} + b \cdot e^{dx}$$

by shifting the latest one along the axis of ordinates on the distance h.

The Sum of Geometrical Dependences with the Free Member

$$f(x) = h + a \cdot x^{c} + b \cdot x^{d}.$$

The graphs of this function can be obtained from the considered above graphs of the sum of geometrical dependences

$$F(x) = a \cdot x^{c} + b \cdot x^{d},$$

by shifting the latest one along the axis of ordinates on the distance h.

Exponential-sine Wave Dependence

$$f(t) = e^{ct}\left(a \cdot \cos(\omega t) + b \cdot \sin(\omega t)\right),\ t > 0,\ \ c\omega \neq 0.$$

The given function can also be represented as

$$f(x) = a \cdot e^{ct} \cdot \cos(\omega t + \varphi) = a \cdot e^{ct} \cdot \sin(\omega t + \psi),$$

where

$$a^2 = A^2 + B^2;\ \tan(\varphi) = -B/A;\ \tan(\psi) = A/B;\ \psi = \varphi + 2\pi/4.$$

Let's introduce also auxiliary parameters

$$T \equiv 2\pi/\omega;\ \ \Omega \equiv |\omega - ic|;\ h \equiv \arg(\omega - ic),$$

where i is the imaginary unit.

The function $f(t)$ is continuous everywhere; it turns into zero in the points $t_k = Tk/2 - \psi/\omega$, it has the maxima in the points $p'_k = Tk - (\varphi + h)/\omega$ and the minima in the points $p''_k = T \cdot (k + 1/2) - (\varphi + h)/\omega$;

$f(p'_k) = (a\omega/\Omega) \cdot \exp(-sp'_k)$; $f(p''_k) = -(a\omega/\Omega) \cdot \exp(-sp''_k)$ $(k = 0, \pm 1, ...)$.

The function $f(t)$ is not periodic, however it turns into zero, and also achieves of the maximal and minimal values over intervals of identical length, equal to T.

The graph of the function $f(t)$ (see Figure A.4.10) is located in the area bounded by graphs of the functions $y = a \cdot e^{ct}$ and $y = -a \cdot e^{ct}$ and has an asymptote, coincided with the axis of abscess. The abscess of the points of a contact of the considered curve with the graph of the function $y = a \cdot e^{ct}$ are equal to $q'_k = Tk - \varphi/\omega$; the abscess of the points of its contact with the graph of the function $y = a \cdot e^{ct}$ are equal to $q''_k = T \cdot (k + 1/2) - \varphi/\omega$. The abscess of the points of inflection are $H_k = Tk/2 - (\varphi + 2h)/\omega$.

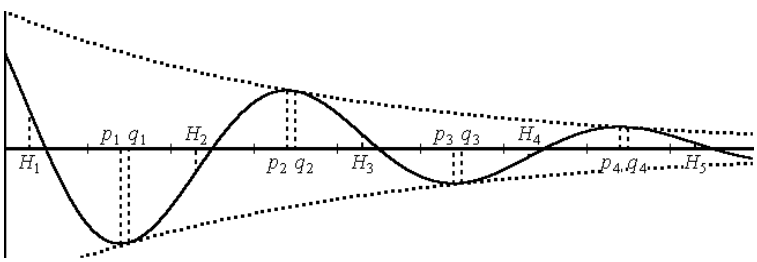


Figure A.4.10. The graph of the functions $y = e^{-ct} \cdot (a \cdot \cos(\omega t) + b \cdot \sin(\omega t))$ (unbroken curve), $y = e^{-ct}$ и $y = -e^{-ct}$ (curves of dots).

Exponential-sine Wave Dependence with the Free Member

$$f(t) = h + e^{ct}(a \cdot \cos(\omega t) + b \cdot \sin(\omega t)),\ t > 0,\ \ c\omega \neq 0.$$

The graphs of this function can be obtained from the considered above graphs of the exponential-sine wave dependence

$$F(t) = e^{ct}(a \cdot \cos(\omega t) + b \cdot \sin(\omega t)),$$

by shifting the latest one along the axis of ordinates on the distance h.

Polynominal Dependence

$$f(x) = \sum_{k=0}^{m} p_k x^k \ .$$

If on the number m there are not imposed restrictions, the function $f(x)$ can have any number of maxima and minima in any points and to accept any values in these points. Therefore to specify any general regularities for the given function is not obviously possible.

The same is possible to say concerning all following functional dependences:

Geometrical-polynominal Dependence

$$f(x) = x^c \cdot \sum_{k=0}^{m} p_k x^k \ ;$$

Exponential-polynominal Dependence

$$f(x) = e^{cx} \cdot \sum_{k=0}^{m} p_k x^k \ ;$$

Logarithmic-polynominal Dependence

$$f(x) = c \cdot \ln\left(\sum_{k=0}^{m} p_k x^k \right);$$

Periodic Dependence

$$f(t) = \sum_{k=0}^{m} \left(A_k \cdot \cos(k\omega t) + B_k \cdot \sin(k\omega t) \right).$$

APPENDIX 5.
GRAPHS OF EXPERIMENTAL INVESTIGATION OF DETERMINISTIC MATHEMATICAL MODELS

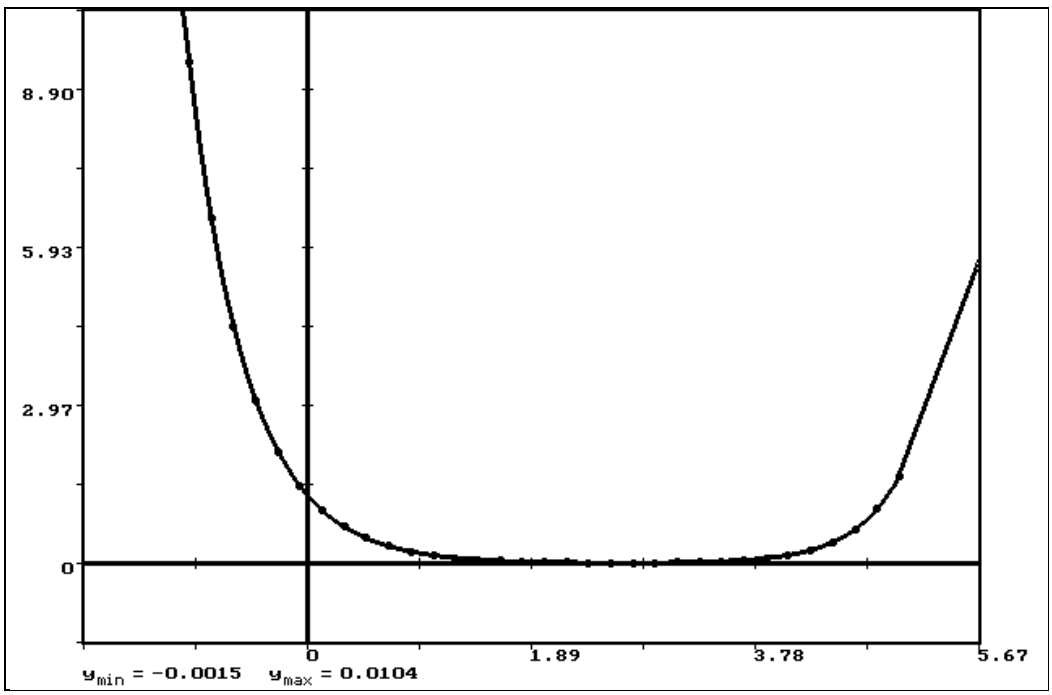


Figure A.5.1. Function I; homogeneous equation; 1D model; classical boundary conditions.

$n_x = 160; T = 0.047\,\text{sec};$

$L = 52; t = 1.95; k = 2.0;$

$\lambda = 2.5; \mu = -2.0; A = 1.5 \cdot 10^{-5}; B = 3.1127;$

$\max\{\Delta\Phi_j\} = 3.8 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.0233.$

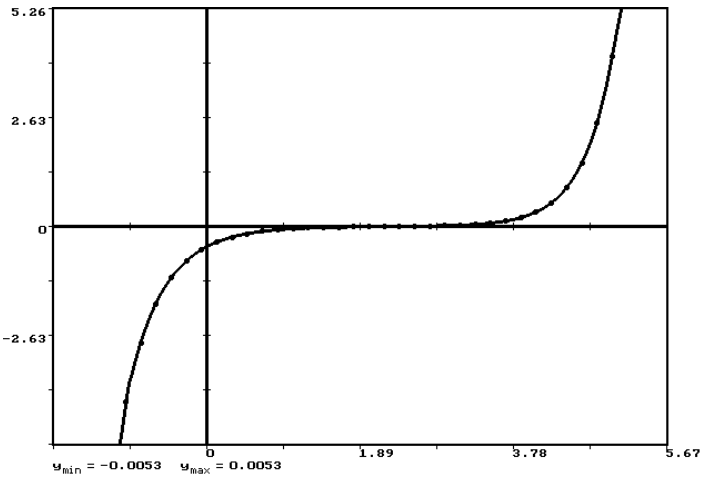


Figure A.5.2. Function I; nonhomogeneous equation; 1D model; classical boundary conditions.

$n_x = 160; T = 0.2\,\text{sec};$
$L = 52; t = 1.95; k = 2.0;$
$\widetilde{\lambda} = 3.0; \widetilde{\mu} = -3.0; \widetilde{A} = 9.2 \cdot 10^{-7}; \widetilde{B} = -0.1145;$
$\max\{\Delta\Phi_j\} = 8.4 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.0382.$

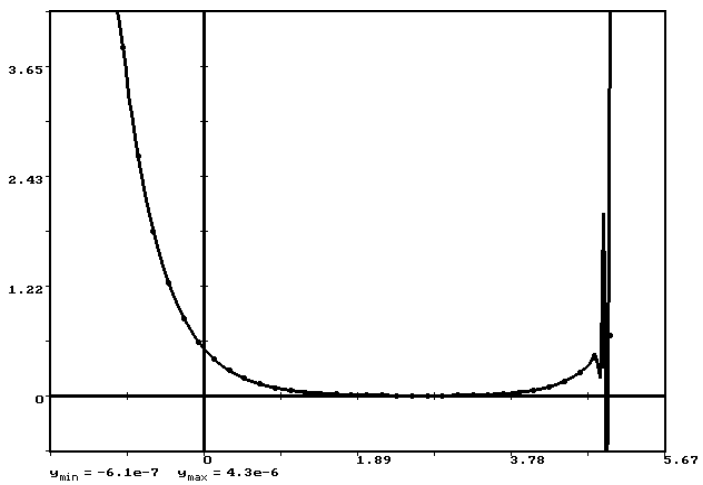


Figure A.5.3. Function I; homogeneous equation 1D model; classical boundary conditions.

$n_x = 160; T = 0.063\,\text{sec};$
$L = 104; t = 3.90; k = 2.0;$
$\lambda = 2.5; \mu = -2.0; A = 1.5 \cdot 10^{-5}; B = 3.1127;$
$\max\{\Delta\Phi_j\} = 4.6 \cdot 10^{-6}; \max\{\Delta\Phi_j / \Phi_j\} = 6.8738.$

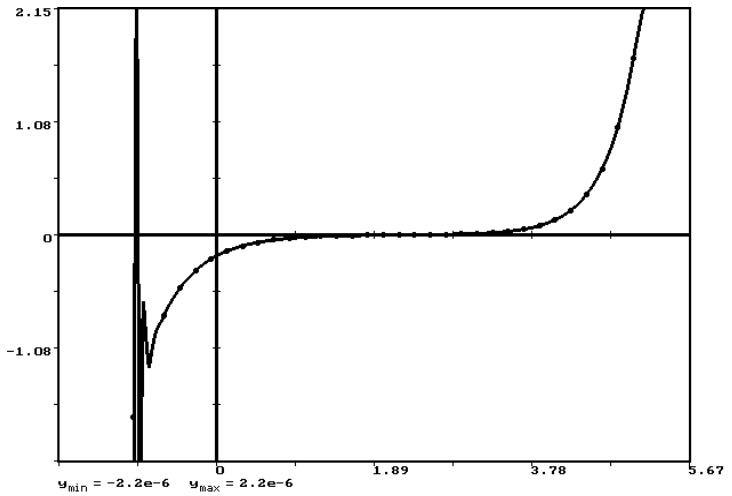


Figure A.5.4. Function I; nonhomogeneous equation 1D model; classical boundary conditions.

$n_x = 160; T = 0.2\,\text{sec};$
$L = 104; t = 3.90; k = 2.0;$
$\widetilde{\lambda} = 3.0; \widetilde{\mu} = -3.0; \widetilde{A} = 9.2 \cdot 10^{-7}; \widetilde{B} = -0.1145;$
$\max\{\Delta\Phi_j\} = 1.1 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 6.0489.$

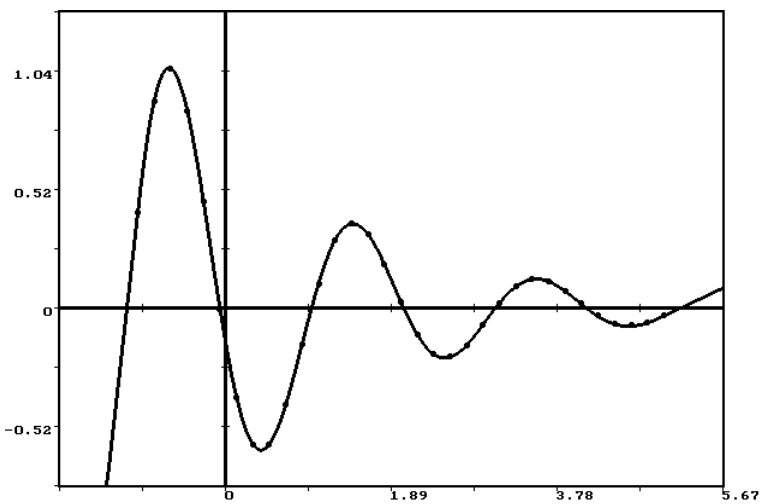


Figure A.5.5. Function II; homogeneous equation 1D model; classical boundary conditions.

$n_x = 1280; T = 2.0\,\text{sec};$
$L = 214; t = 1.00; k = 2.0;$
$\omega = 3.0; s = -0.5; A = -8.1213; B = -41.881;$
$\max\{\Delta\Phi_j\} = 0.0037; \max\{\Delta\Phi_j / \Phi_j\} = 0.1883.$

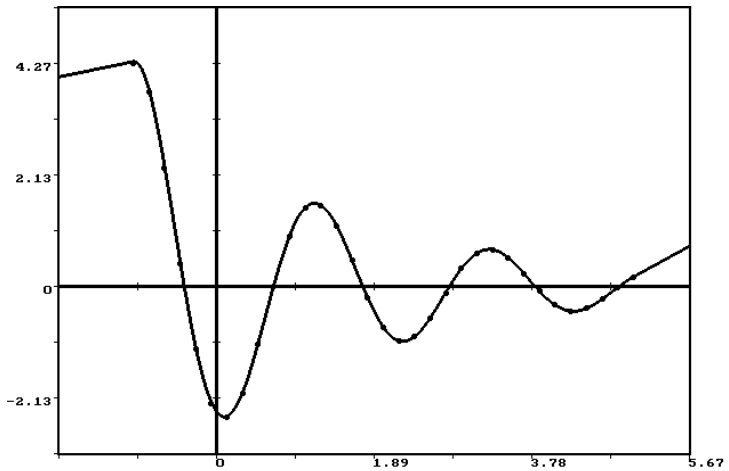


Figure A.5.6. Function II; nonhomogeneous equation; 1D model; classical boundary conditions.

$n_x = 1280; T = 3.5\,\text{sec};$
$L = 214; t = 1.00; k = 2.0;$
$\widetilde{\omega} = 3.5; \widetilde{s} = -0.3; \widetilde{A} = 24.306; \widetilde{B} = -8.3140;$
$\max\{\Delta\Phi_j\} = 0.0390; \max\{\Delta\Phi_j / \Phi_j\} = 2.0382.$

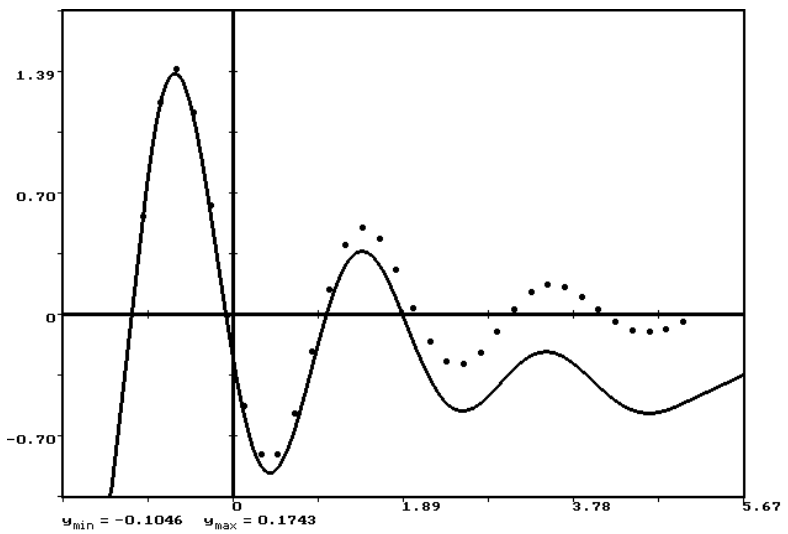


Figure A.5.7. Function II; homogeneous equation 1D model; classical boundary conditions.

$n_x = 1280; T = 2.0\,\text{sec};$
$L = 321; t = 1.50; k = 2.0;$
$\omega = 3.0; s = -0.5; A = -8.1213; B = -41.881;$
$\max\{\Delta\Phi_j\} = 0.0470; \max\{\Delta\Phi_j / \Phi_j\} = 17.343.$

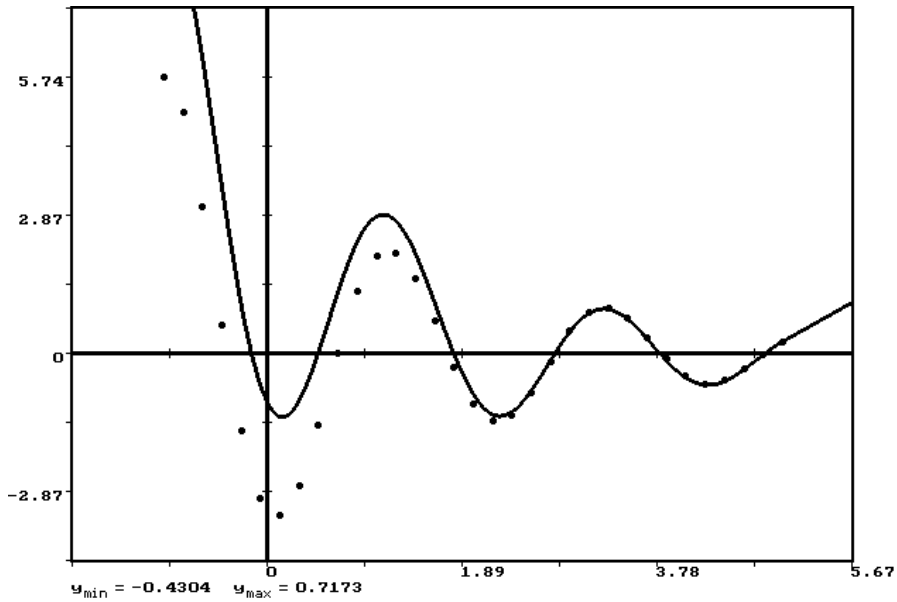


Figure A.5.8. Function II; nonhomogeneous equation; 1D model; classical boundary conditions.

$n_x = 1280; T = 3.5\,\text{sec};$
$L = 321; t = 1.50; k = 2.0;$
$\widetilde{\omega} = 3.5; \widetilde{s} = -0.3; \widetilde{A} = 24.306; \widetilde{B} = -8.3140;$
$\max\{\Delta\Phi_j\} = 0.3207; \max\{\Delta\Phi_j / \Phi_j\} = 173.12.$

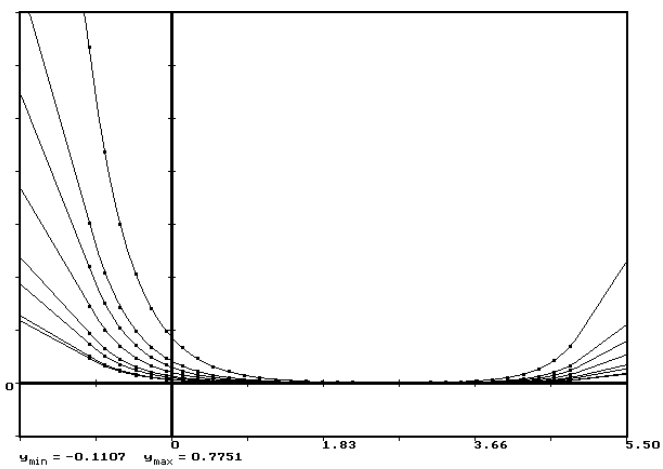


Figure A.5.9. Function I; homogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 756; T = 1.1\,\text{sec};$
$n_x = 53; n_y = 13;$
$L = 36; t = 1.51; k = 2.0;$
$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\max\{\Delta\Phi_j\} = 0.0195; \max\{\Delta\Phi_j / \Phi_j\} = 0.1760.$

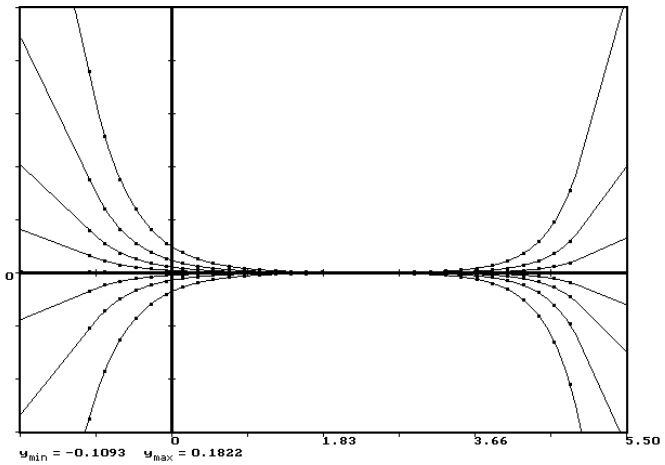


Figure A.5.10. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 742; T = 2.6\text{sec};$
$n_x = 52; n_y = 13;$
$L = 36; t = 1.53; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\max\{\Delta\Phi_j\} = 0.0039; \max\{\Delta\Phi_j / \Phi_j\} = 0.6809.$

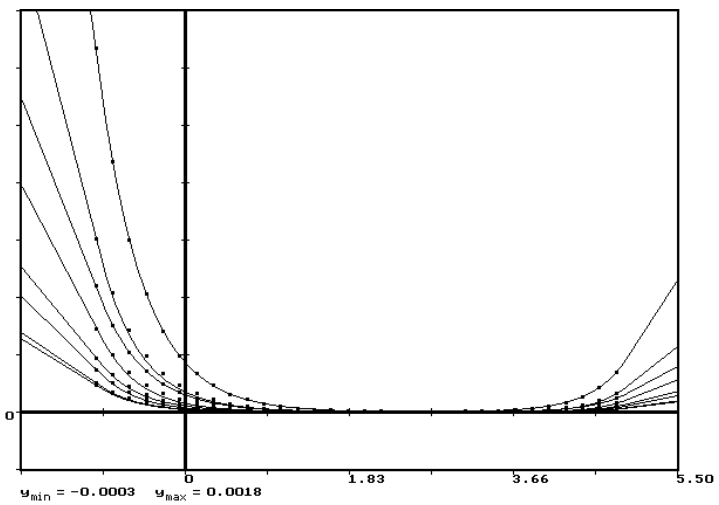


Figure A.5.11. Function I; homogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 756; T = 1.1\text{sec};$
$n_x = 53; n_y = 13;$
$L = 72; t = 3.031; k = 2.0;$
$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\max\{\Delta\Phi_j\} = 4.6 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.1760.$

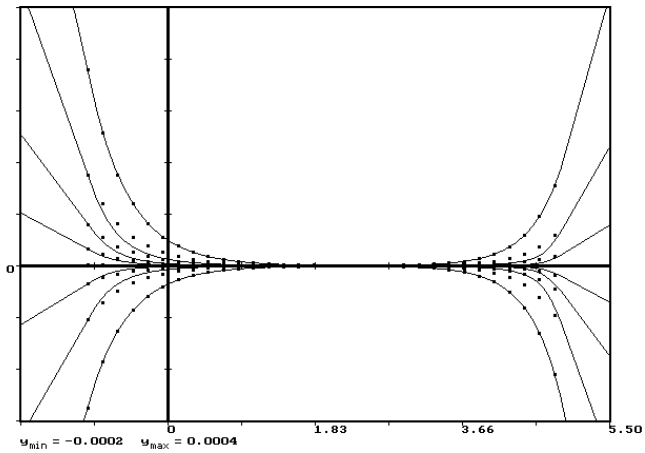


Figure A.5.12. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 742; T = 2.6\text{sec};$
$n_x = 52; n_y = 13;$
$L = 72; t = 3.07; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\max\{\Delta\Phi_j\} = 8.4 \cdot 10^{-6}; \max\{\Delta\Phi_j / \Phi_j\} = 0.3121.$

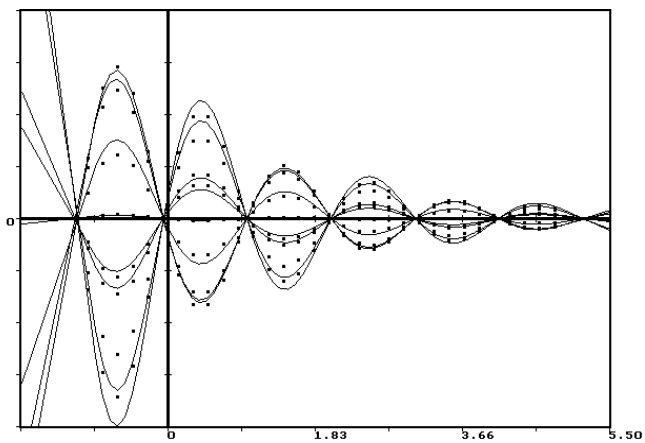


Figure A.5.13. Function I; homogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 1584; T = 0.8\text{sec};$
$n_x = 65; n_y = 23;$
$L = 12; t = 0.30; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\max\{\Delta\Phi_j\} = 0.5189; \max\{\Delta\Phi_j / \Phi_j\} = 8.8661.$

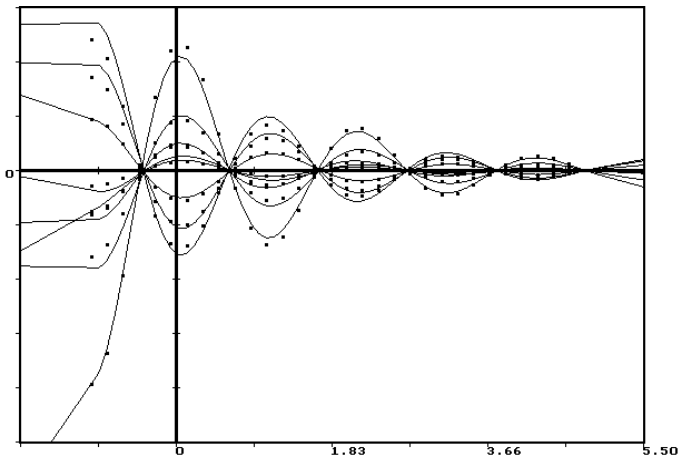


Figure A.5.14. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 1560; T = 1.6\text{sec};$

$n_x = 64; n_y = 23;$

$L = 12; t = 0.31; k = 2.0;$

$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$

$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$

$\max\{\Delta\Phi_j\} = 1.7264; \max\{\Delta\Phi_j / \Phi_j\} = 87.688.$

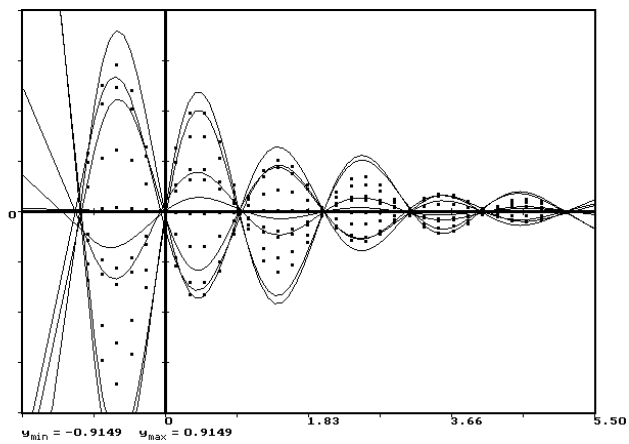


Figure A.5.15. Function I; homogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 1584; T = 0.8\text{sec};$

$n_x = 65; n_y = 23;$

$L = 24; t = 0.61; k = 2.0;$

$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$

$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$

$\max\{\Delta\Phi_j\} = 0.4565; \max\{\Delta\Phi_j / \Phi_j\} = 91.681.$

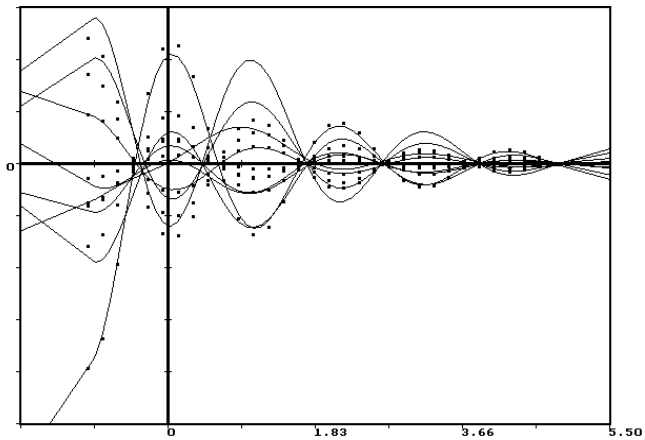


Figure A.5.16. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; method of decomposition of operator.

$N = 1560; T = 1.6\text{sec};$
$n_x = 64; n_y = 23;$
$L = 24; t = 0.62; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\max\{\Delta\Phi_j\} = 1.4428; \max\{\Delta\Phi_j / \Phi_j\} = 428.19.$

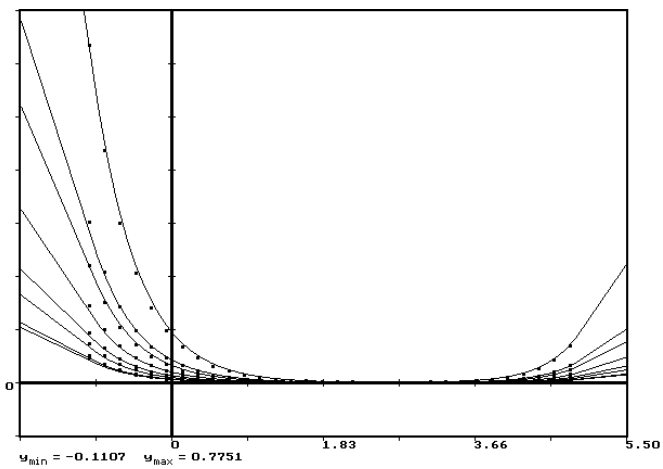


Figure A.5.17. Function I; homogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 756; T = 28\text{sec};$
$n_x = 53; n_y = 13;$
$L = 36; t = 1.51; k = 2.0;$
$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\max\{\Delta\Phi_j\} = 0.0042; \max\{\Delta\Phi_j / \Phi_j\} = 0.0485.$

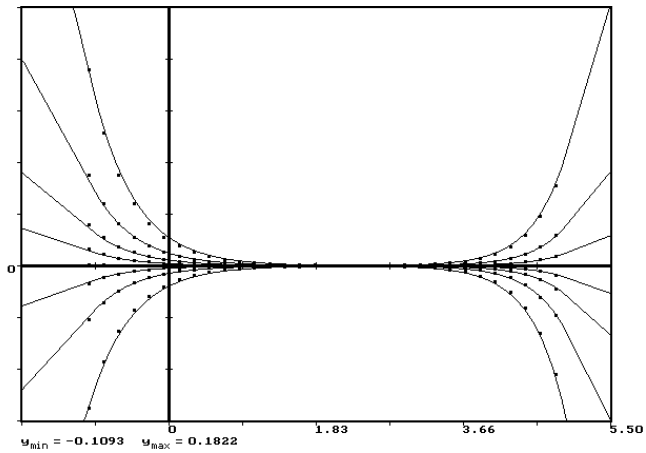


Figure A.5.18. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 742; T = 47\text{sec};$
$n_x = 52; n_y = 13;$
$L = 36; t = 1.53; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\max\{\Delta\Phi_j\} = 0.0008; \max\{\Delta\Phi_j / \Phi_j\} = 1.0804.$

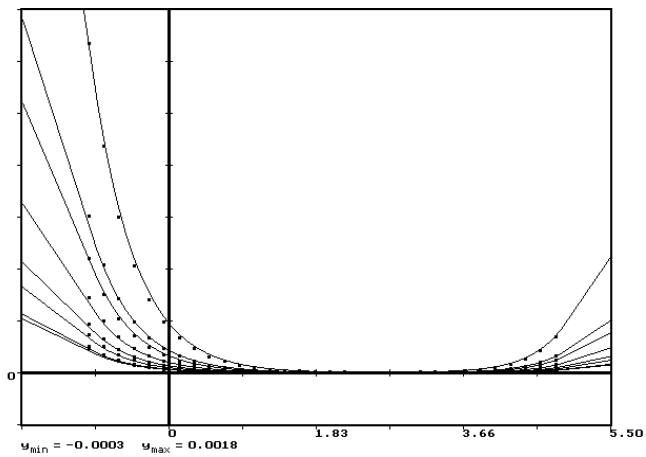


Figure A.5.19. Function I; homogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 756; T = 13\text{sec};$
$n_x = 53; n_y = 13;$
$L = 72; t = 3.03; k = 2.0;$
$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\max\{\Delta\Phi_j\} = 2.6 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.6877.$

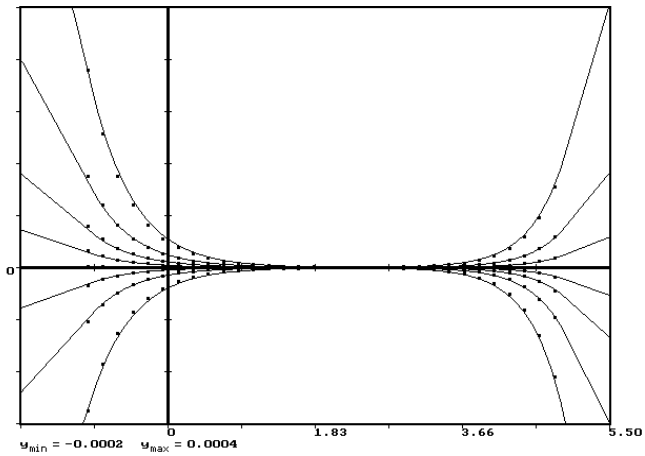


Figure A.5.20. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 742; T = 18\text{sec};$
$n_x = 52; n_y = 13;$
$L = 72; t = 3.07; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\max\{\Delta\Phi_j\} = 2.0 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.9910.$

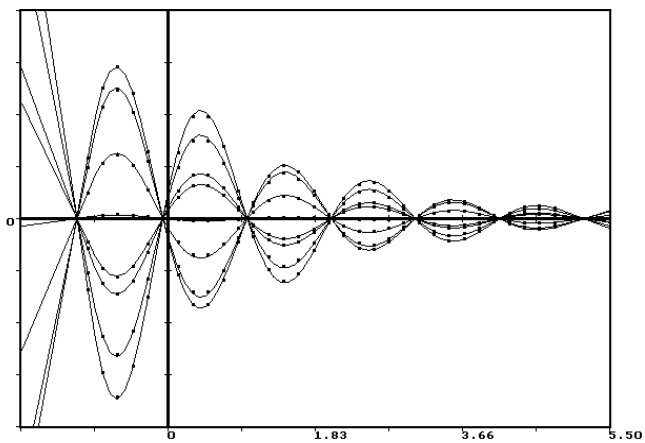


Figure A.5.21. Function I; homogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 1584; T = 29\text{sec};$
$n_x = 65; n_y = 23;$
$L = 12; t = 0.30; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\max\{\Delta\Phi_j\} = 0.0365; \max\{\Delta\Phi_j / \Phi_j\} = 2.5718.$

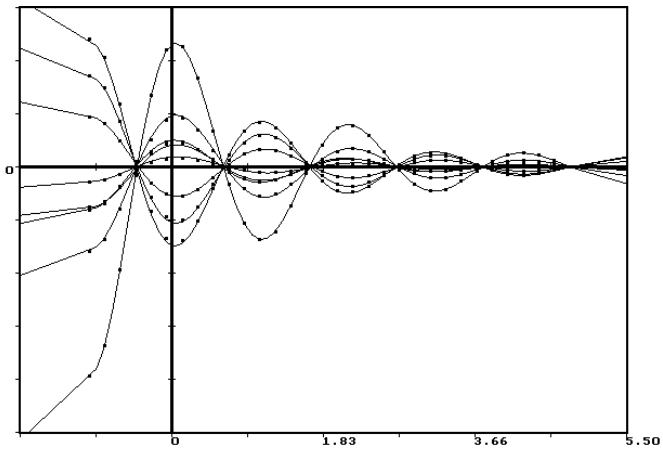


Figure A.5.22. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 1560; T = 49\text{sec};$
$n_x = 64; n_y = 23;$
$L = 12; t = 0.31; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\max\{\Delta\Phi_j\} = 0.2922; \max\{\Delta\Phi_j / \Phi_j\} = 53.821.$

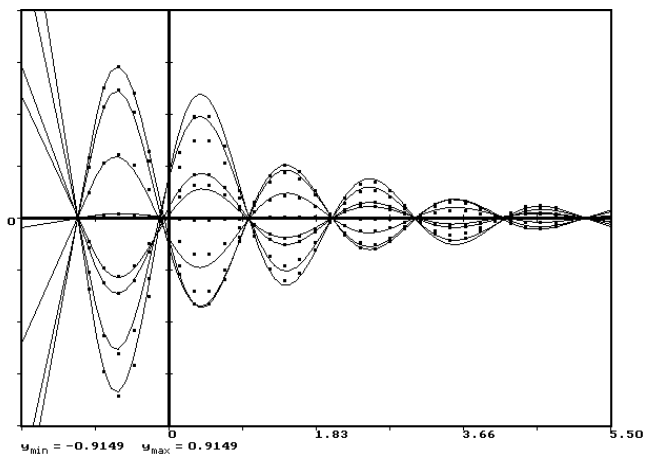


Figure A.5.23. Function I; homogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 1584; T = 27\text{sec};$
$n_x = 65; n_y = 23;$
$L = 24; t = 0.61; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\max\{\Delta\Phi_j\} = 0.0990; \max\{\Delta\Phi_j / \Phi_j\} = 111.12.$

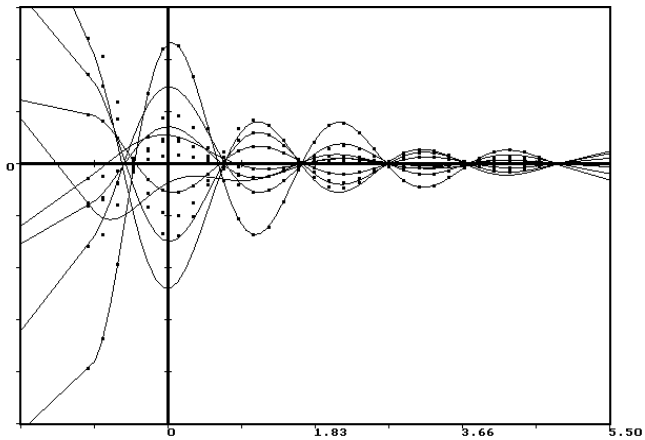


Figure A.5.24. Function I; nonhomogeneous equation; 2D model; classical boundary conditions; Zeidel method.

$N = 1560; T = 49\text{sec};$
$n_x = 64; n_y = 23;$
$L = 24; t = 0.62; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\max\{\Delta\Phi_j\} = 1.3274; \max\{\Delta\Phi_j / \Phi_j\} = 415.20.$

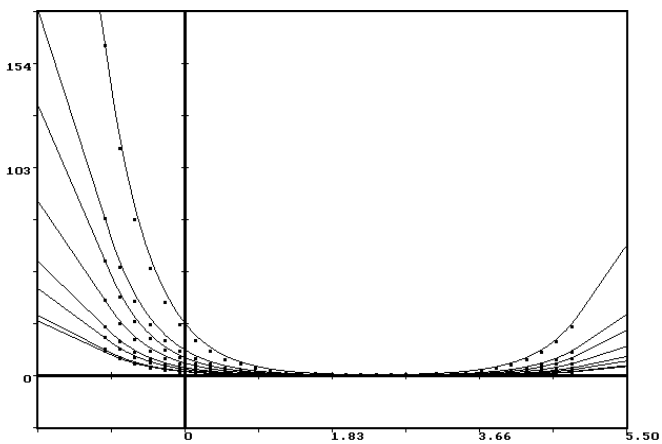


Figure A.5.25. Function I; homogeneous equation; 3D model; classical boundary conditions; method of decomposition of operator.

$N = 7344; T = 5.4\text{sec};$
$n_x = 47; n_y = 16; n_z = 8;$
$L = 10; t = 0.64; k = 2.0;$
$\lambda_1 = 2.0; \mu_1 = -2.0; A_1 = 0.0002; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\lambda_3 = 1.1; \mu_3 = -0.9; A_3 = 0.2637; B_3 = 8.2525;$
$\max\{\Delta\Phi_j\} = 6.3123; \max\{\Delta\Phi_j / \Phi_j\} = 0.5242.$

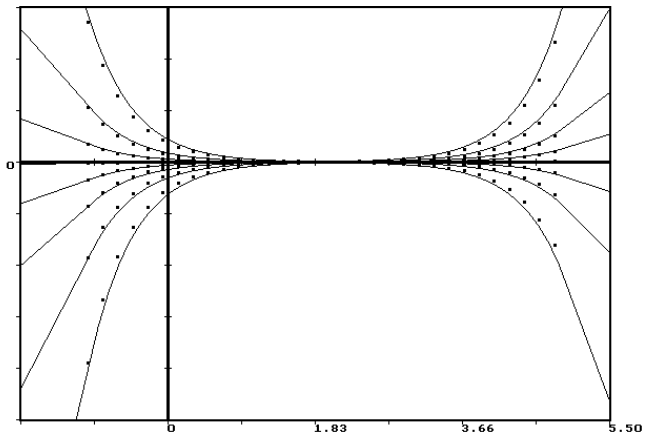


Figure A.5.26. Function I; nonhomogeneous equation; 3D model; classical boundary conditions; method of decomposition of operator.

$N = 7191; T = 14\text{sec};$
$n_x = 46; n_y = 16; n_z = 8;$
$L = 10; t = 0.64; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\widetilde{\lambda}_3 = 0.7; \widetilde{\mu}_3 = -0.7; \widetilde{A}_3 = 0.2577; \widetilde{B}_3 = -3.0151;$
$\max\{\Delta\Phi_j\} = 1.4122; \max\{\Delta\Phi_j / \Phi_j\} = 0.6808.$

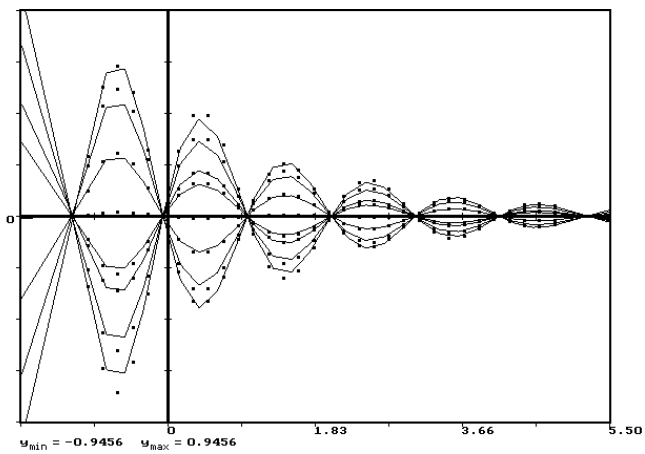


Figure A.5.27. Function I; homogeneous equation; 3D model; classical boundary conditions; method of decomposition of operator.

$N = 3780; T = 5.9\text{sec};$
$n_x = 26; n_y = 13; n_z = 9;$
$L = 20; t = 0.05; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\omega_3 = 1.7; s_3 = -0.3; A_3 = 0.5959; B_3 = -1.0252;$
$\max\{\Delta\Phi_j\} = 0.0952; \max\{\Delta\Phi_j / \Phi_j\} = 1.7371.$

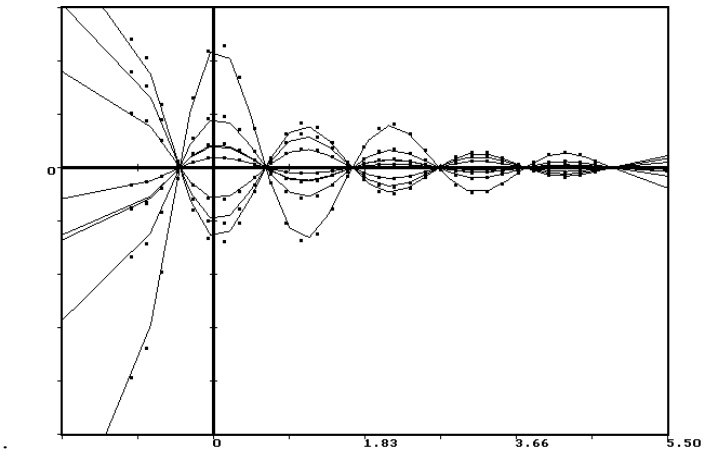


Figure A.5.28. Function I; nonhomogeneous equation; 3D model; classical boundary conditions; method of decomposition of operator.

$N = 3640; T = 13\text{sec};$
$n_x = 25; n_y = 13; n_z = 9;$
$L = 20; t = 0.05; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\widetilde{\omega}_3 = 2.6; \widetilde{s}_3 = -0.1; \widetilde{A}_3 = 0.6534; \widetilde{B}_3 = -0.4413;$
$\max\{\Delta\Phi_j\} = 9.5009; \max\{\Delta\Phi_j / \Phi_j\} = 0.5775.$

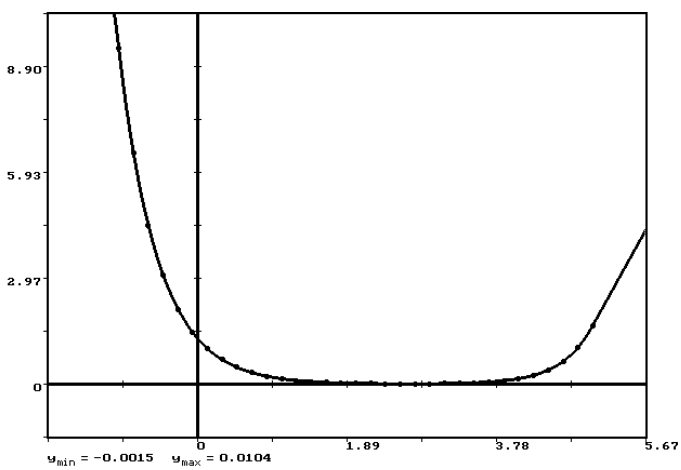


Figure A.5.29. Function I; homogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 160; T = 0.06\,\text{sec};$
$L = 52; t = 1.95; k = 2.0;$
$\lambda = 2.5; \mu = -2.0; A = 1.5 \cdot 10^{-5}; B = 3.1127;$
$\max\{\Delta\Phi_j\} = 4.6 \cdot 10^{-6}; \max\{\Delta\Phi_j / \Phi_j\} = 0.0047.$

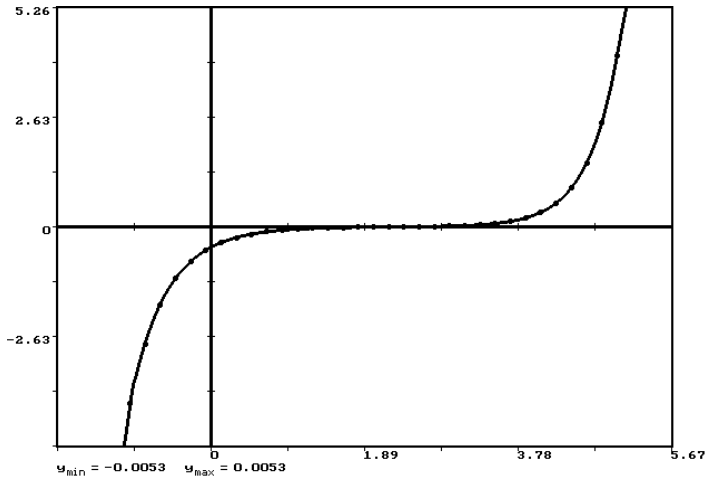


Figure A.5.30. Function I; nonhomogeneous equation; 1D model; nonclassical boundary conditions. 1D model; nonclassical boundary conditions.

$n_x = 160; T = 0.2\,\text{sec};$

$L = 52; t = 1.95; k = 2.0;$

$\tilde{\lambda} = 3.0; \tilde{\mu} = -3.0; \tilde{A} = 9.2 \cdot 10^{-7}; \tilde{B} = -0.1145;$

$\max\{\Delta\Phi_j\} = 8.4 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.0382.$

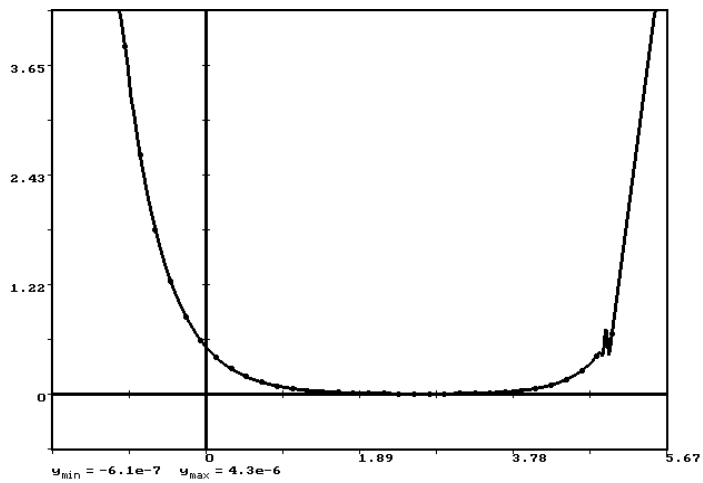


Figure A.5.31. Function I; homogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 160; T = 0.2\,\text{sec};$

$L = 104; t = 3.90; k = 2.0;$

$\lambda = 2.5; \mu = -2.0; A = 1.5 \cdot 10^{-5}; B = 3.1127;$

$\max\{\Delta\Phi_j\} = 1.4 \cdot 10^{-8}; \max\{\Delta\Phi_j / \Phi_j\} = 0.0334.$

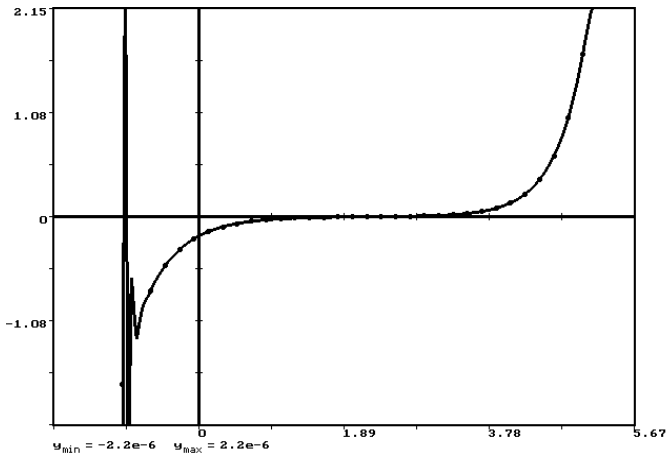


Figure A.5.32. Function I; nonhomogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 160; T = 0.4\,\text{sec};$
$L = 104; t = 3.90; k = 2.0;$
$\widetilde{\lambda} = 3.0; \widetilde{\mu} = -3.0; \widetilde{A} = 9.2 \cdot 10^{-7}; \widetilde{B} = -0.1145;$
$\max\{\Delta\Phi_j\} = 1.1 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 6.0489.$

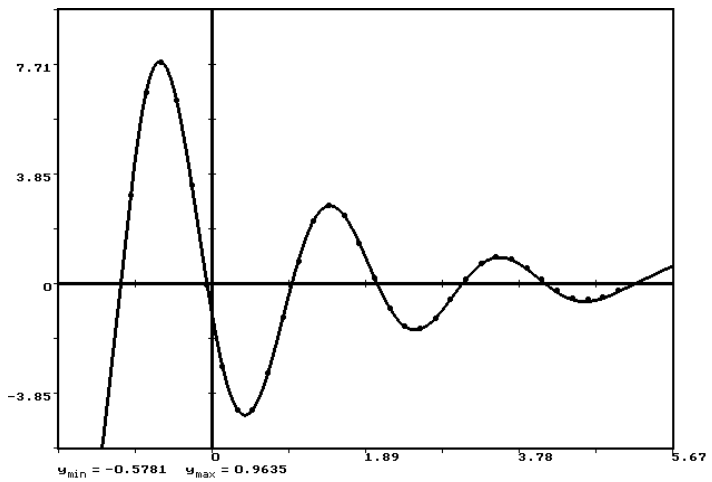


Figure A.5.33. Function II; homogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 1280; T = 1.9\,\text{sec};$
$L = 107; t = 0.50; k = 2.0;$
$\omega = 3.0; s = -0.5; A = -0.8121; B = -4.1881;$
$\max\{\Delta\Phi_j\} = 0.0062; \max\{\Delta\Phi_j / \Phi_j\} = 0.3970.$

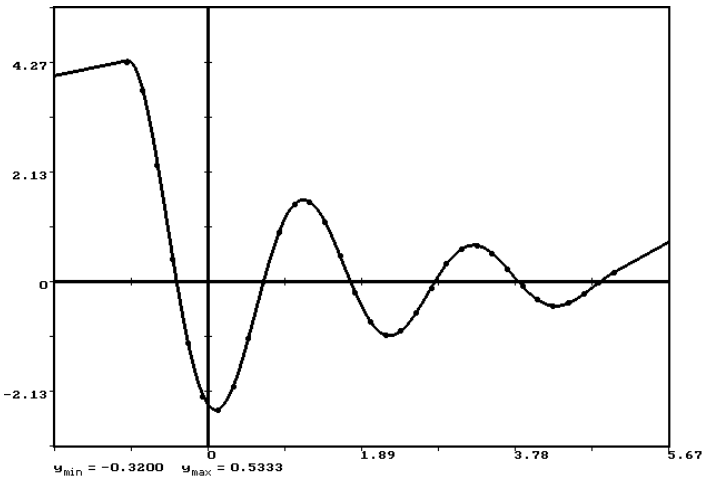


Figure A.5.34. Function II; nonhomogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 1280; T = 6.8\,\text{sec};$
$L = 214; t = 1.00; k = 2.0;$
$\widetilde{\omega} = 3.5; \widetilde{s} = -0.3; \widetilde{A} = 2.4306; \widetilde{B} = -0.8314;$
$\max\{\Delta\Phi_j\} = 0.0039; \max\{\Delta\Phi_j / \Phi_j\} = 2.0382.$

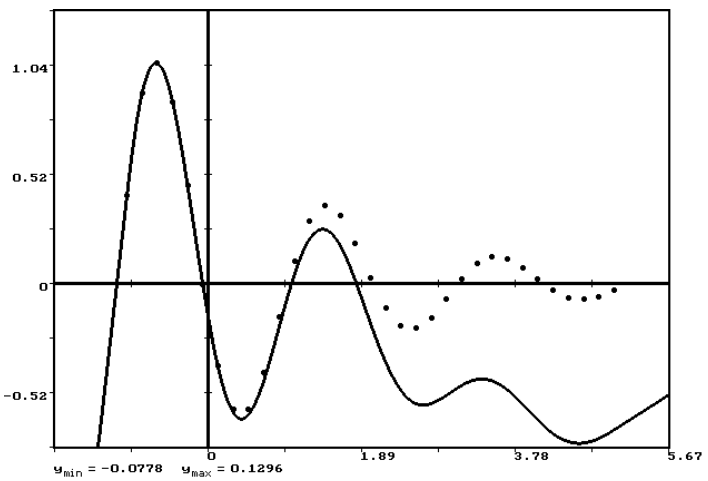


Figure A.5.35. Function II; nonhomogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 1280; T = 3.8\,\text{sec};$
$L = 214; t = 1.00; k = 2.0;$
$\omega = 3.0; s = -0.5; A = -0.8121; B = -4.1881;$
$\max\{\Delta\Phi_j\} = 0.0684; \max\{\Delta\Phi_j / \Phi_j\} = 35.489.$

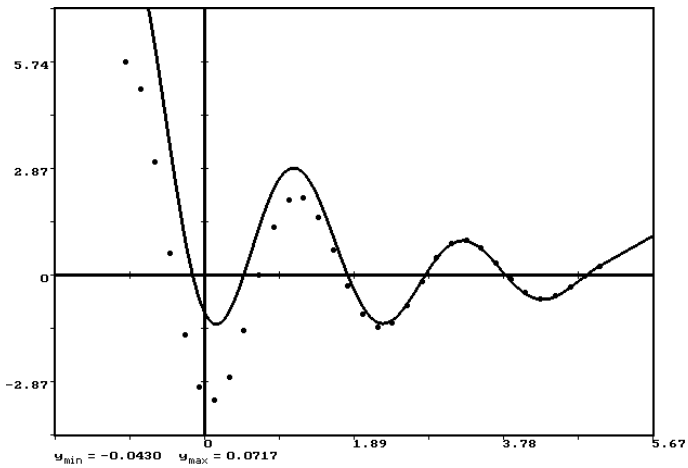


Figure A.5.36. Function II; nonhomogeneous equation; 1D model; nonclassical boundary conditions.

$n_x = 1280; T = 10.2\,\text{sec};$
$L = 321; t = 1.50; k = 2.0;$
$\widetilde{\omega} = 3.5; \widetilde{s} = -0.3; \widetilde{A} = 2.4306; \widetilde{B} = -0.8314;$
$\max\{\Delta\Phi_j\} = 0.0321; \max\{\Delta\Phi_j / \Phi_j\} = 173.12.$

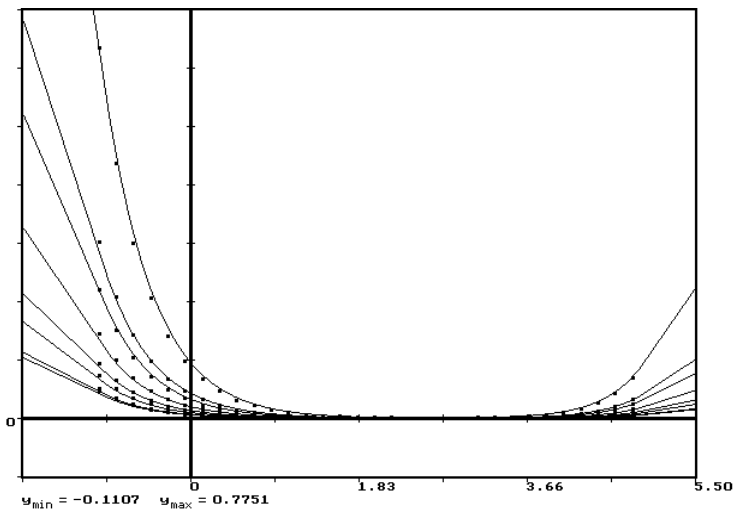


Figure A.5.37. Function I; homogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 756; T = 1.1\text{sec};$
$n_x = 53; n_y = 13;$
$L = 36; t = 1.51; k = 2.0;$
$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\max\{\Delta\Phi_j\} = 0.0195; \max\{\Delta\Phi_j / \Phi_j\} = 0.1760.$

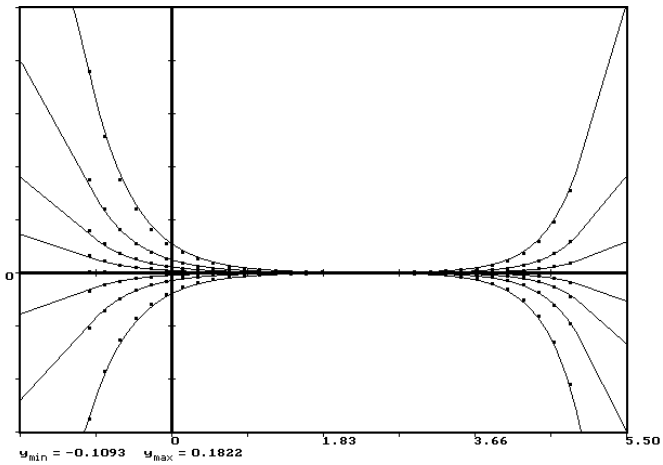


Figure A.5.38. Function I; nonhomogeneous equation;2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 742; T = 2.6\text{sec};$

$n_x = 52; n_y = 13;$

$L = 36; t = 1.53; k = 2.0;$

$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$

$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$

$\max\{\Delta\Phi_j\} = 0.0039; \max\{\Delta\Phi_j / \Phi_j\} = 0.6809.$

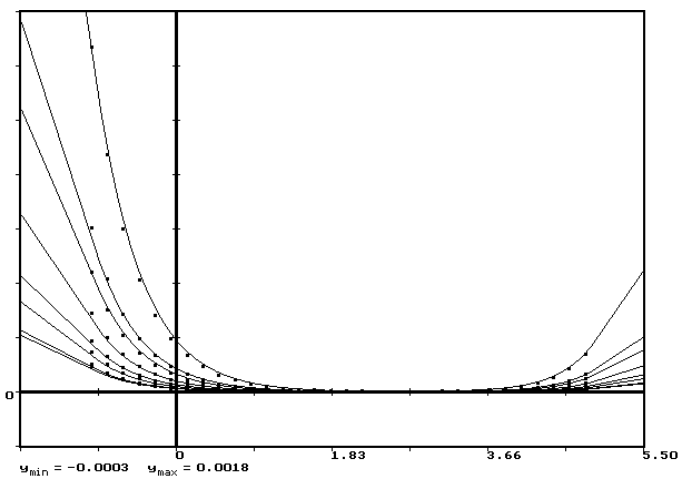


Figure A.5.39. Function I; homogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 756; T = 1.1\text{sec};$

$n_x = 53; n_y = 13;$

$L = 72; t = 3.03; k = 2.0;$

$\lambda_1 = 2.5; \mu_1 = -2.0; A_1 = 1.5 \cdot 10^{-5}; B_1 = 3.1127;$

$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$

$\max\{\Delta\Phi_j\} = 4.6 \cdot 10^{-5}; \max\{\Delta\Phi_j / \Phi_j\} = 0.1760.$

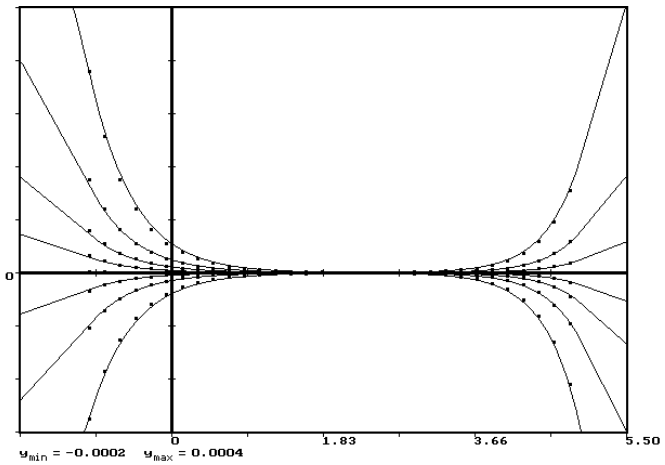


Figure A.5.40. Function I; nonhomogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 742; T = 2.6\text{sec};$

$n_x = 52; n_y = 13;$

$L = 72; t = 3.07; k = 2.0;$

$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$

$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$

$\max\{\Delta\Phi_j\} = 8.4 \cdot 10^{-6}; \max\{\Delta\Phi_j / \Phi_j\} = 0.3121.$

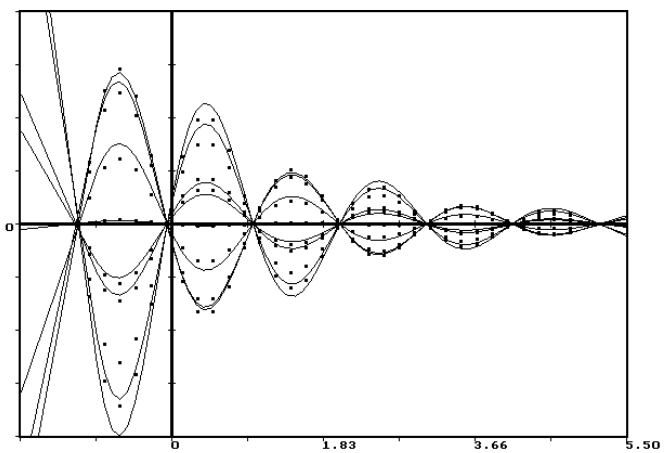


Figure A.5.41. Function I; homogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 1584; T = 0.8\text{sec};$

$n_x = 65; n_y = 23;$

$L = 12; t = 0.30; k = 2.0;$

$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$

$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$

$\max\{\Delta\Phi_j\} = 0.5189; \max\{\Delta\Phi_j / \Phi_j\} = 8.8661.$

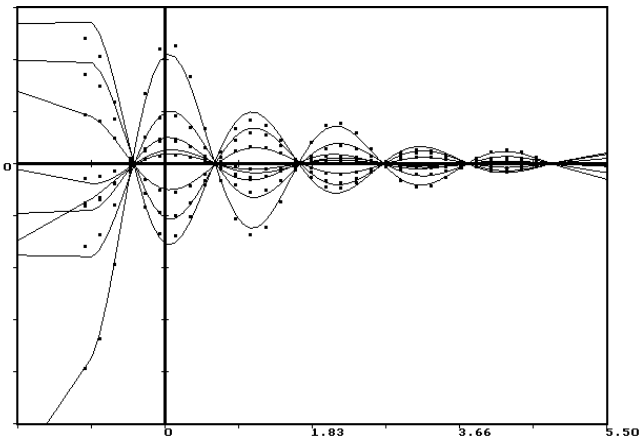


Figure A.5.42. Function I; nonhomogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 1560; T = 1.6\text{sec};$
$n_x = 64; n_y = 23;$
$L = 12; t = 0.31; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\max\{\Delta\Phi_j\} = 1.7264; \max\{\Delta\Phi_j / \Phi_j\} = 87.688.$

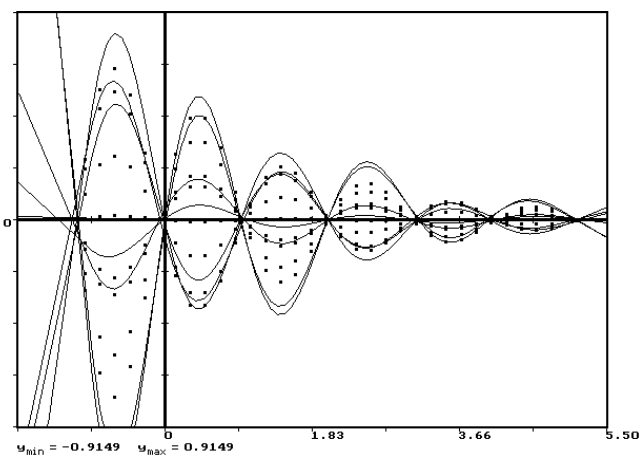


Figure A.5.43. Function I; homogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 1584; T = 0.8\text{sec};$
$n_x = 65; n_y = 23;$
$L = 24; t = 0.61; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\max\{\Delta\Phi_j\} = 0.4565; \max\{\Delta\Phi_j / \Phi_j\} = 91.681.$

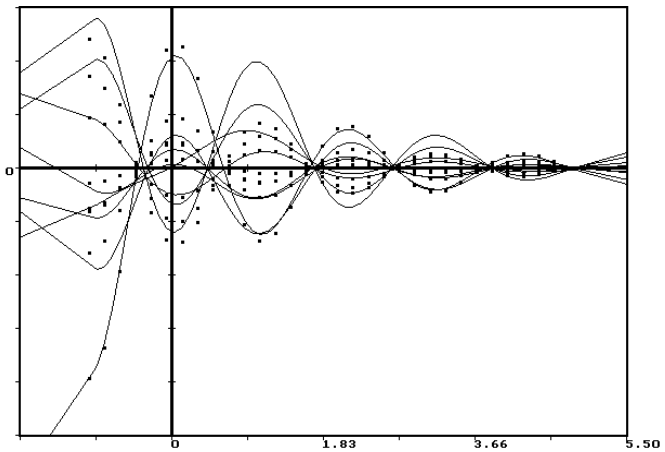


Figure A.5.44. Function I; nonhomogeneous equation; 2D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 1560; T = 1.6\text{sec};$
$n_x = 64; n_y = 23;$
$L = 24; t = 0.62; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\max\{\Delta\Phi_j\} = 1.4428; \max\{\Delta\Phi_j / \Phi_j\} = 428.19.$

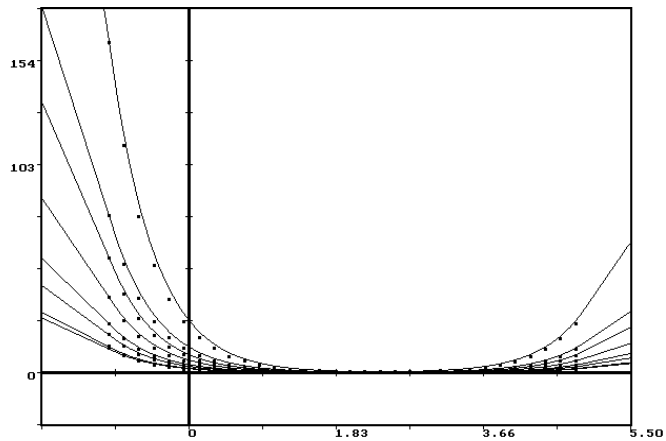


Figure A.5.45. Function I; homogeneous equation; 3D model; nonclassical boundary conditions; nonclassical boundary conditions; method of decomposition of operator.

$N = 7344; T = 5.4\text{sec};$
$n_x = 47; n_y = 16; n_z = 8;$
$L = 10; t = 0.64; k = 2.0;$
$\lambda_1 = 2.0; \mu_1 = -2.0; A_1 = 0.0002; B_1 = 3.1127;$
$\lambda_2 = 1.6; \mu_2 = -1.3; A_2 = 0.0164; B_2 = 6.7827;$
$\lambda_3 = 1.1; \mu_3 = -0.9; A_3 = 0.2637; B_3 = 8.2525;$
$\max\{\Delta\Phi_j\} = 6.3123; \max\{\Delta\Phi_j / \Phi_j\} = 0.5242.$

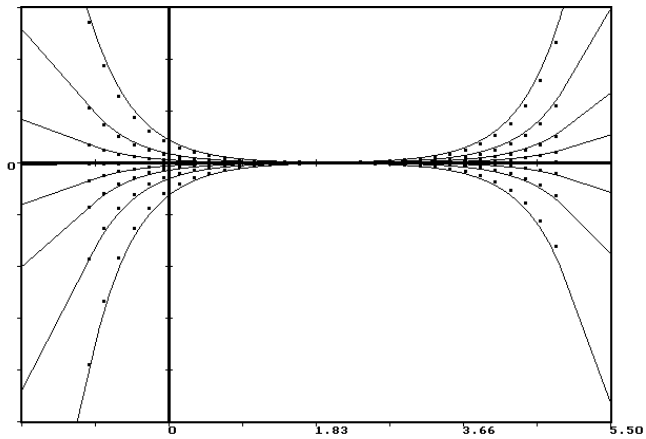


Figure A.5.46. Function I; nonhomogeneous equation; 3D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 7191; T = 14\text{sec};$
$n_x = 46; n_y = 16; n_z = 8;$
$L = 10; t = 0.64; k = 2.0;$
$\widetilde{\lambda}_1 = 3.0; \widetilde{\mu}_1 = -3.0; \widetilde{A}_1 = 9.2 \cdot 10^{-7}; \widetilde{B}_1 = -0.1145;$
$\widetilde{\lambda}_2 = 2.1; \widetilde{\mu}_2 = -2.1; \widetilde{A}_2 = 0.0011; \widetilde{B}_2 = -0.5414;$
$\widetilde{\lambda}_3 = 0.7; \widetilde{\mu}_3 = -0.7; \widetilde{A}_3 = 0.2577; \widetilde{B}_3 = -3.0151;$
$\max\{\Delta\Phi_j\} = 1.4122; \max\{\Delta\Phi_j / \Phi_j\} = 0.6808.$

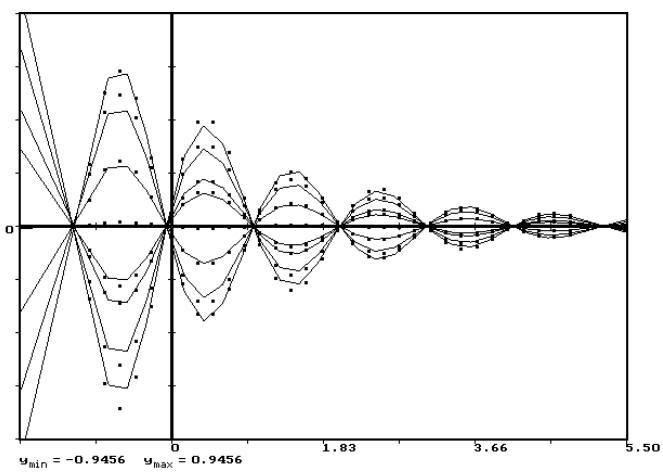


Figure A.5.47. Function I; homogeneous equation; 3D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 3780; T = 6.0\text{sec};$
$n_x = 26; n_y = 13; n_z = 9;$
$L = 20; t = 0.05; k = 2.0;$
$\omega_1 = 3.0; s_1 = -0.5; A_1 = -0.8121; B_1 = -4.1881;$
$\omega_2 = 2.2; s_2 = -0.3; A_2 = -0.9330; B_2 = -1.7304;$
$\omega_3 = 1.7; s_3 = -0.3; A_3 = 0.5959; B_3 = -1.0252;$
$\max\{\Delta\Phi_j\} = 0.0952; \max\{\Delta\Phi_j / \Phi_j\} = 1.7371.$

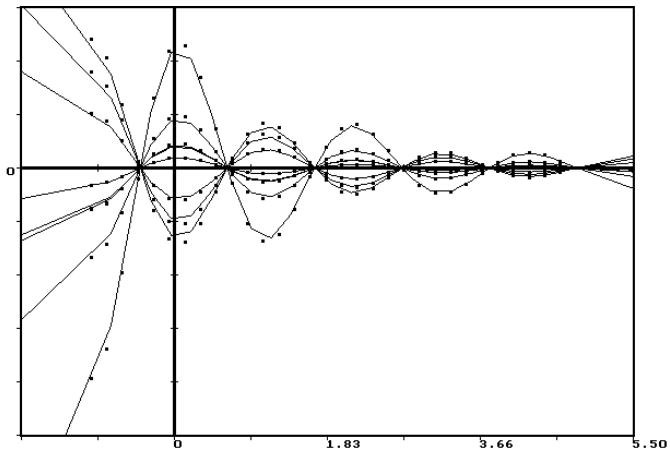


Figure A.5.48. Function I; nonhomogeneous equation; 3D model; nonclassical boundary conditions; method of decomposition of operator.

$N = 3640; T = 13\text{sec};$
$n_x = 25; n_y = 13; n_z = 9;$
$L = 20; t = 0.05; k = 2.0;$
$\widetilde{\omega}_1 = 3.5; \widetilde{s}_1 = -0.3; \widetilde{A}_1 = 2.4306; \widetilde{B}_1 = -0.8314;$
$\widetilde{\omega}_2 = 3.1; \widetilde{s}_2 = -0.2; \widetilde{A}_2 = 0.1270; \widetilde{B}_2 = -0.3748;$
$\widetilde{\omega}_3 = 2.6; \widetilde{s}_3 = -0.1; \widetilde{A}_3 = 0.6534; \widetilde{B}_3 = -0.4413;$
$\max\{\Delta\Phi_j\} = 9.5009; \max\{\Delta\Phi_j / \Phi_j\} = 0.5775.$

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