# 2.3 DYNAMIC MODELS-DISTRIBUTED PARAMETER SYSTEMS

- Distributed parameter models, as their name suggests, **incorporate the spatial variation of states** within the balance volume.

- They account for situations where the scalar field of the intensive quantities is **both a function of time and position**.

- This could be a concentration, volume-specific internal energy or temperature.

- What this means is that the application of the general conservation equations leads to models which are represented by **partial differential equations (PDEs)** in one, two or three spatial dimensions.

- **EXAMPLE (DPS model of a simple packed bed tubular catalytic reactor**)

Process system:

- Consider a tubular reactor completely filled with catalyst and with ideal plug flow.

- A first-order catalytic reaction A→P takes place in an incompressible fluid phase.
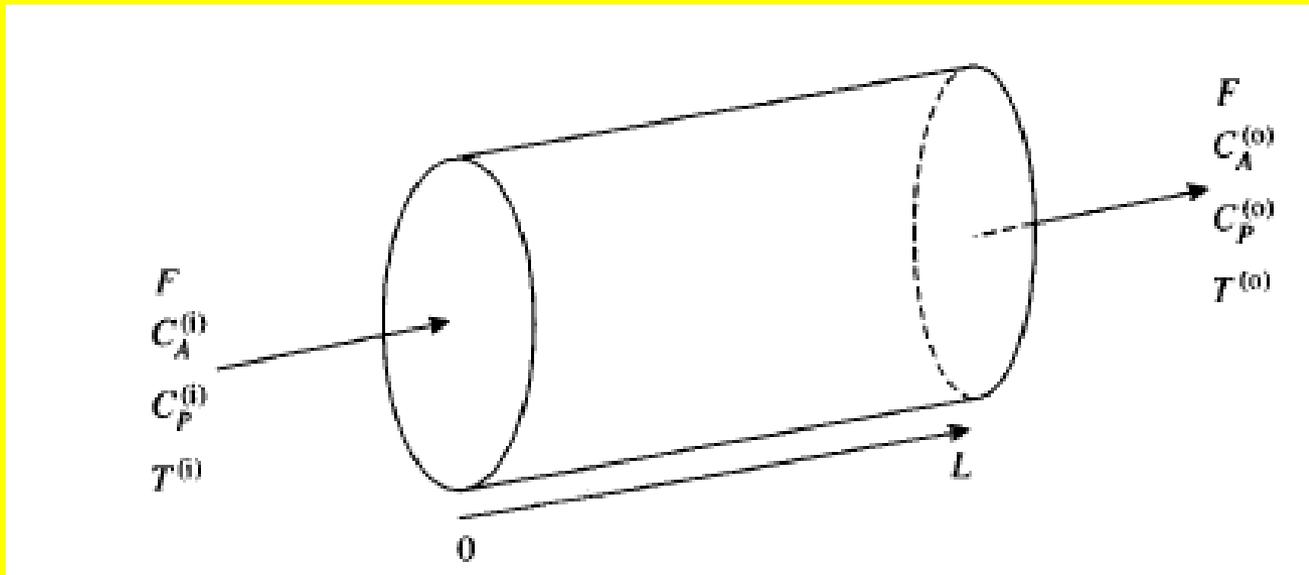
Modeling goal

''Describe the behavior of the reactor (concentration and temperature) for temperature control purposes.''

- From the problem description above, we may extract the following modeling assumptions which will be generally valid for any further model.

Assumptions

- Al. Plug flow is assumed in the reactor, which has constant volume.

- A2. A first-order reaction A →P takes place.

- A3. An incompressible (liquid) phase is present as a bulk phase.

- A4. A solid phase catalyst is present which is uniformly distributed.

Modelling of Distributed Parameter Systems

<u>Balance Volumes</u>

- In the case of DPS, we define a **local co-ordinate system and then carry out balances over a representative element of that system.**

- we apply three commonly used approaches, which are normally **dictated by the geometry of the system**. These are:

- **Rectangular co-ordinates**; typically Cartesian co-ordinates in terms of the directions x, y and z.

- **Cylindrical co-ordinates**; where the key dimensions are radius (r), angle (θ) and length (z).

- **Spherical co-ordinates**; where two angles (θ and Φ) are given, plus a radius r.

- It is **up to the modeler to decide** which geometry suits the actual physical system.

- It is usually the case that **most physical systems assume one of these geometric shapes**, or the region of interest approximates to a slab, cylinder or sphere.

- Once the geometry is decided, then it is necessary to carry out the balance of mass, energy or momentum **over a representative infinitesimal volume of the space**.

- This can take the form of a "**slice**" or "**shell**" in the region of interest.
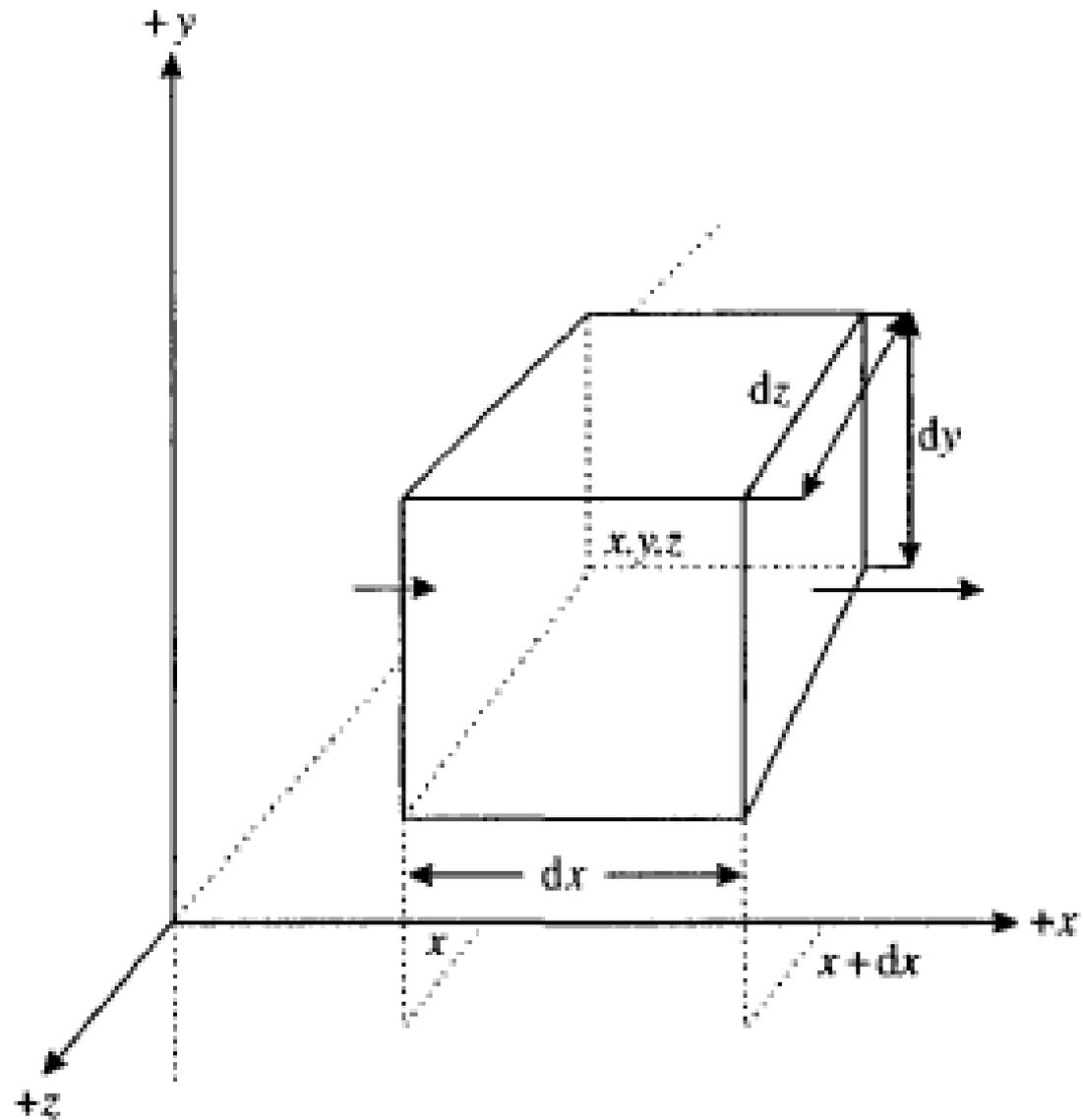
Balance volume in rectangular co-ordinates.

- In order to develop the balance equations of the DPS model, we have to derive a special case of this general equation taking into account :

  - **the geometry of the system** to select the co-ordinate system,

  -**Modelling assumptions** that define the general terms in the equation.

- Thereafter, **the constitutive equations** should also be given, based on the modelling assumptions.

- The following example of the **packed bed plug flow catalytic reactor** will illustrate how a distributed parameter model can be derived.

- In order to simplify the form of the equations, we add some more simplifying assumptions.

- Assumptions additional to the ones listed as 1-4 are the following:

A5 . The reactor is **uniformly distributed in its cross-section**, i.e. no radial diffusion or convection takes place.

A6. Constant **physico-chemical properties**.

A7. The heat transfer through the reactor wall is considered, but the **outer temperature is assumed to be constant**, T_W

Balance volumes

- A single volume encapsulating **the whole reactor**. This is now a distributed system.

- The **rectangular co-ordinate system** is chosen.

Model equations

- Variables

$$0 \leq x \leq L, \quad 0 \leq t, \quad C_A(x,t), \quad T(x,t), \quad \hat{U}(x,t),$$

- Where x is the spatial coordinate in axial direction, L is the length of the reactor, t is the time, C_A is the reactant concentration (i.e. volume-specific component mass), U is the volume-specific internal energy and T is the temperature.

- **Component mass balance:**

$$\frac{\partial C_A}{\partial t} = D \frac{\partial^2 C_A}{\partial x^2} - F \frac{\partial C_A}{\partial x} - r_A,$$

- where F is the mass flowrate of the inert incompressible fluid, D is the diffusion coefficient and r_A is the reaction rate.

Energy balance:

$$\frac{\partial \hat{U}}{\partial t} = \kappa \frac{\partial^2 \hat{U}}{\partial x^2} - F \frac{\partial \hat{U}}{\partial x} - \Delta H r_A - q_{tr},$$

- where q_{tr} is the heat transfer rate, K the heat diffusion coefficient and ΔH is the reaction enthalpy.

Constitutive equations:

- Potential relation:

$$\hat{U} = c_P \rho T,$$

- where cp is the constant specific energy and ρ is the density

Reaction rate relation

$$r_A = k_0 e^{-E/RT} C_A,$$

- where k_o is the pre-exponential factor, E is the activation energy, and R is the universal gas constant.

Transfer rate relation:

$$q_{tr} = K(T - T_w),$$

where K is the heat transfer coefficient

Boundary Conditions and Initial Conditions

- The specification of boundary conditions and initial conditions is **extremely important in DPS models**.

- There are several different types of boundary conditions which are applied to these systems.

- In order to have a well-posed model, we need to develop the **governing equations as well as specifying initial conditions** for time dependent problems as well as **appropriate boundary conditions** for the system.

Boundary Conditions

- Boundary conditions are specified for all time **on each of the boundaries** of the problem.

- In a heat exchange problem, this might mean setting the incoming fluid temperature T and concentration C_A at x = 0. It can be a function of time **T(0, t)** and **C_A(0, t)** hence act as **forcing functions or disturbances on the system**.

- Boundary conditions appear in three major forms which are important to consider.

- These forms are commonly called first or **Dirichlet**, second or **Neumann** and **Robbins** or third type conditions.
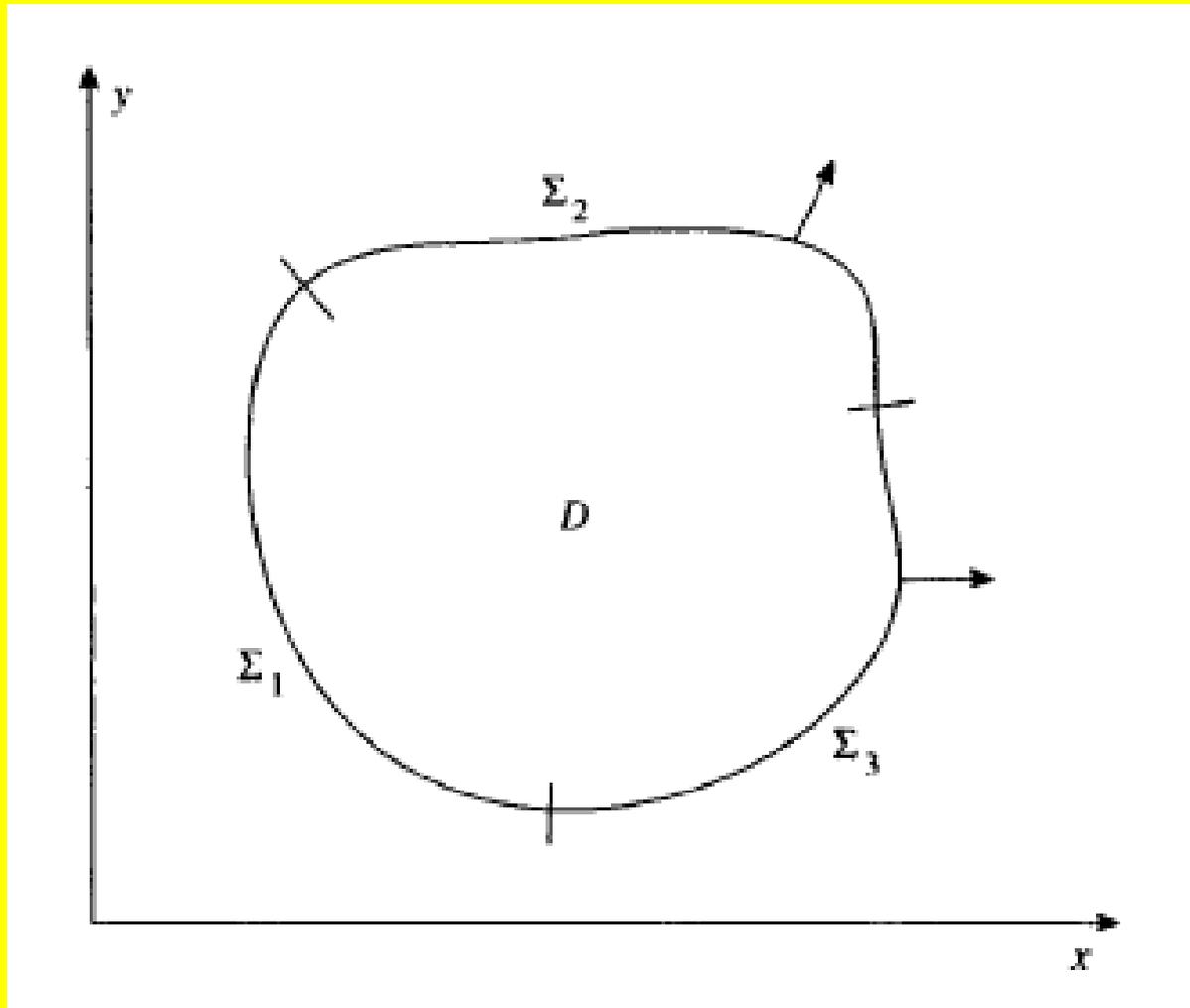
Boundary regions for three types of conditions

For the general equation in (X,Y), we can identify three distinct boundary conditions.

- (a) **The Dirichlet problem**, *where the value of the function is specified on the* boundary, i.e.

$$\Phi = f(x, y) \quad \text{on} \quad \Sigma_1.$$

- (b) **The Neumann problem**, *where the normal derivative is specified, i.e.*

$$\frac{\partial \Phi}{\partial n} = g(x, y) \quad \text{on} \quad \Sigma_2$$

(c) **The Robbins problem**, third type or mixed condition, where we have

$$\alpha(x, y)\Phi + \beta(x, y)\frac{\partial \Phi}{\partial n} = \gamma(x, y) \quad \text{on } \Sigma_3$$

with

$$\alpha(x, y) > 0, \quad \beta(x, y) > 0 \text{ for } (x, y) \in D.$$

Assumptions Relevant to the Boundary Conditions

Conditions on the physical boundaries of the system

- For a mass transfer situation, we could interpret the Dirichlet condition as setting a concentration on the boundary,

$$C(0, t) = C_0.$$

- The Neumann condition **would be equivalent to a flux at the boundary**. For example, for a perfectly isolated boundary at x= 0 orthogonal to the *x co-ordinate* direction, the mass flux should be equal to zero, so that

$$\frac{\partial C_A}{\partial x}(0, t) = 0$$

- The third type of boundary condition would be equivalent to **convective mass transfer** across the boundary.

- If again we assume a boundary orthogonal to the X co-ordinate direction and assume component mass transfer driven by the difference between the concentration within the system on the boundary at x= x_M with $C_A(X_M, t)$ and a given fixed **outer concentration C*** we have

$$\frac{\partial C_A}{\partial x}(x_M, t) = K\left(C^* - C_A(x_M, t)\right)$$

Number of boundary conditions

- The number of independent boundary conditions along a given co-ordinate direction depends **on the order of the partial derivative** operator in that direction.

- The **number of independent boundary conditions along a co-ordinate direction should be equal to the order** of the corresponding partial derivative operator .

- Therefore, if we have **no diffusion but only convection in a direction we should specify one condition**; otherwise, **with diffusion we must have two boundary conditions**.

- The two boundary conditions **can be on one or both sides** of the interval of the co-ordinate direction.

- Care needs to be taken that two or more boundary conditions are not set simultaneously for a specified boundary region.

Infinitely large balance volumes

- Special boundary conditions are used to express the fact that the balance volume is very large or infinitely large in a co-ordinate direction.

- We may set the size of the balance volume in that direction and

  ❑ set the concentration of the reactants to zero using Dirichlet conditions **at the boundary**;

  ❑ specify that all convective and diffusive flow is zero at that boundary using Neumann conditions.

- **EXAMPLE (Derivation of the initial and boundary conditions for the simple packed bed tubular catalytic reactor)**

- In order to simplify the form of the initial and boundary conditions, we add some more simplification assumptions.

Assumptions additional to the ones listed as 1-7 are:

- A8. The initial distribution of component A and the initial temperature in the reactor is **uniformly constant**.

- A9. The reactor is very long in the x co-ordinate direction to enable **full conversion**.

Initial and boundary conditions

- Initial conditions

$$C_A(x, 0) = C_A^*, \quad T(x, 0) = T^*.$$

- Boundary conditions

$$\frac{\partial C_A}{\partial x}(L, 0) = 0, \quad C_A(0, t) = C_A^{(i)},$$

$$\frac{\partial T}{\partial x}(L, 0) = 0, \quad T(0, t) = T^{(i)},$$

- Where C_A^i and T^i are the **inlet concentration** and the inlet temperature, while C_A^* and T^* are the **initial** concentrations and temperature, respectively.

- Note that **two boundary conditions are needed because of the presence of the diffusion** in both of the balance equations.

- The first condition at the outlet of the reactor expresses the **fact that the reactor is very long and the reaction is fully completed before the flow exits**

Initial Conditions

- Initial conditions set the values of the states at the initial time (typically t = 0) for the whole of the region of interest.

- For example, in the DPS model of the tubular catalytic reactor we needed to set the initial fluid temperature and concentration along the length of the reactor. These conditions can be given as

$$T(x, 0) = f_1(x),$$
$$C_A(x, 0) = f_2(x),$$

- Where f_1 and f_2 are given functions in space.

Modelling Assumptions and their Effect on the Model Equations

- The most important modelling assumptions which affect the model equations of a DPS are summarized below.

- The assumptions are grouped according to the model element or property they reflect.

Shape of the balance volumes

-The shape of the balance volumes **determines the co-ordinate system adopted**. This affects **the mathematical form of the conservation balances** in their convection and diffusion terms.

Size of the balance volumes

-Very large balance volumes (in any of their co-ordinate directions) may call for **special boundary conditions**.

Phases in the process system

-Solid phase in a balance volume **implies the absence of convection**.

Flow conditions

-Plug flow conditions imply **convection in the direction of the flow with uniform flowrate in every other direction**. The flow conditions determine the vector field describing the convective flow.

Mixing conditions

- Perfect mixing in any of the co-ordinate direction implies no diffusion and **uniform distribution of the intensive properties** in that direction.

EXAMPLES OF DISTRIBUTED PARAMETER MODELLING

1) DPS Model of a Double-pipe Heat Exchanger

- The mathematical model of a double-pipe heat exchanger shows a lot of similarities to the model of the tubular catalytic rector we have seen before.

- The process system consists of **a double pipe heated from outside by condensing saturated steam**.

Process system

- Consider a simple ID double-pipe exchanger where a liquid stream is being heated by condensing saturated steam at a temperature, T_s.
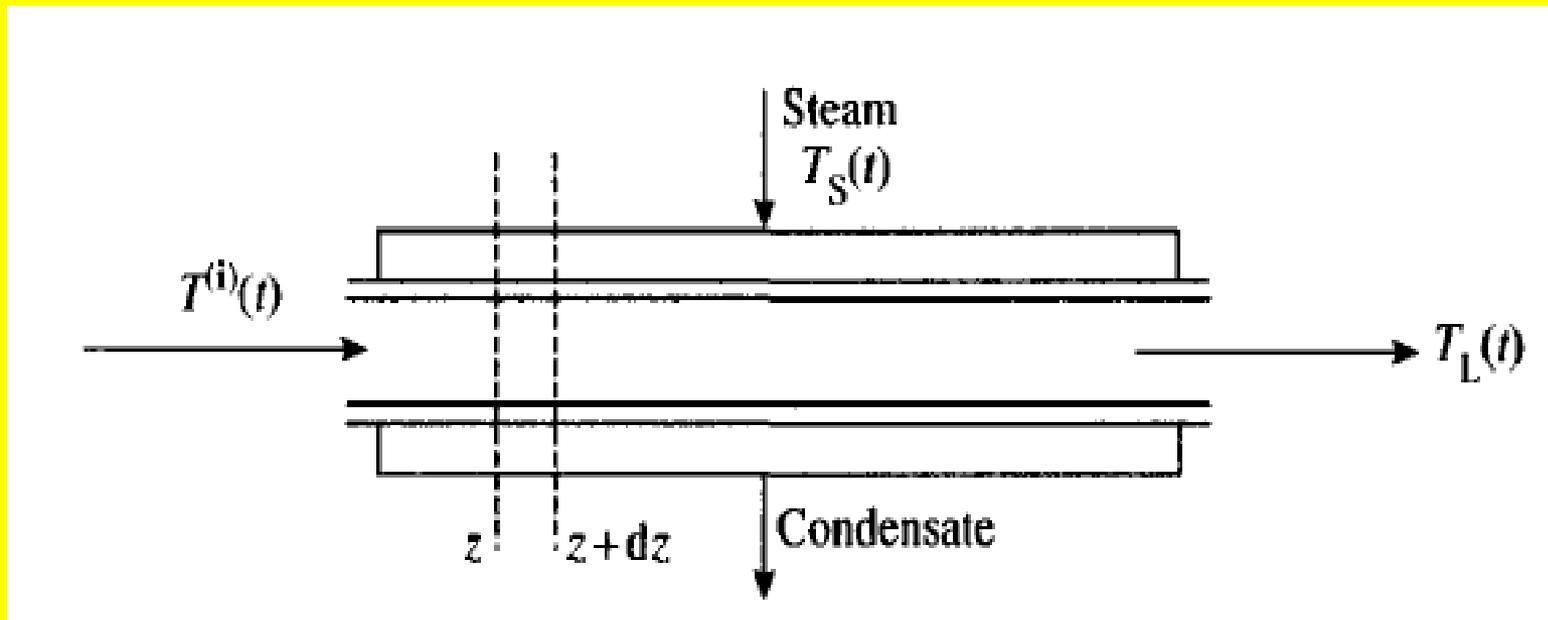
- Fluid enters at temperature $T_L(O, t)$ and exits at $T_L(L, t)$. Heat transfer takes place between the steam (T_s) and the wall (T_w) and then to the fluid $T_L(Z, t)$

- The spatial variation is related to the fluid temperature whilst the steam temperature is a **"lumped" variable, Ts**.

Assumptions

- A 1. The overall mass (volume) of the liquid as well as that of the wall is constant.

- A2. No diffusion takes place.

- A3. Steam temperature reacts instantaneously to supply changes.

- A4. Heat transfer coefficients are constant.

- A5. Specific heats and densities are constant.

- A6. Time delays are negligible for fluid.

- A7. Liquid is in plug flow.

- **Balance volumes**

- Two volumes is considered and for the fluid and the wall, respectively, both of them are distributed. The rectangular co-ordinate system is chosen.

- **Model equations**

- Variables

$$0 \leq z \leq L, \quad 0 \leq t, \quad T_{\mathrm{L}}(z, t), \quad T_{\mathrm{w}}(z, t),$$

- Where z is the axial co-ordinate along the tube and L is the tube length.

- Energy balance for the liquid

$$\rho_L A_f c_L \frac{\partial T_L}{\partial t} = -u \rho_L A_f c_L \frac{\partial T_L}{\partial z} + h_L A_L (T_w - T_L).$$

- Energy balance for the wall

$$M_w c_w \frac{\partial T_w}{\partial t} = h_s A_s (T_s - T_w) - h_L A_L (T_w - T_L),$$

where

ρ_L fluid density $[kg/m^3]$

A_f flow area $[m^2]$

c_L fluid heat capacity $[J/kg\,K]$

u fluid velocity $[m/s]$

h_L fluid heat transfer coefficient $[W/m^2\,K]$

A_L internal tube area per length of tube [m^2/m]

M_w mass of tube per length [kg/m]

c_w metal heat capacity [J/kg K]

A_s external tube area [m^2/m]

h_s steam side heat transfer coefficient [W/m^2 K]

- **Initial conditions**

$$T_L(z, 0) = f_1(z),$$
$$T_w(z, 0) = f_2(z).$$

- **Boundary condition**

$$T_L(0, t) = T^{(i)}(t) \quad \text{for all } t \geq 0,$$

- Where T^i *is the inlet concentration of the liquid*

- We can simplify the above PDEs by defining some time constants for the system.

- For example,

  - $\tau_L = \frac{\rho_L c_L A_f}{h_L A_L}$ (characteristic fluid heating time),

  - $\tau_{sw} = \frac{M_w c_w}{h_s A_s}$ (steam to wall thermal constant),

  - $\tau_{wL} = \frac{M_w c_w}{h_L A_s}$ (wall to fluid thermal constant).

- Modified equations are then

$$\frac{\partial T_L}{\partial t} = -u\frac{\partial T_L}{\partial z} + \frac{1}{\tau_L}(T_w - T_L),$$

$$\frac{\partial T_w}{\partial t} = \frac{1}{\tau_{sw}}(T_s - T_w) - \frac{1}{\tau_{wL}}(T_w - T_L).$$

- There are some interesting key steps in developing the DPS model above which are as follows:

  1. Only **one spatial co-ordinate** is needed **because of the plug flow** assumption.

  2. We have substituted the constitutive equations into the balance equations. The transfer rate relation was simply substituted as the only source term. potential **relation $U = cp\rho T$ with constant physico-chemical properties has been substituted into the energy conservation equations** .

- 3. Note that ***T_s is a function of time only** and acts as a forcing function on the* system.

- 4. The model equations are ***coupled PDEs since the wall temperature (Tw) depends on the fluid temperature (T_L).***

- 5. A particular steady-state solution profile to the above model is shown below
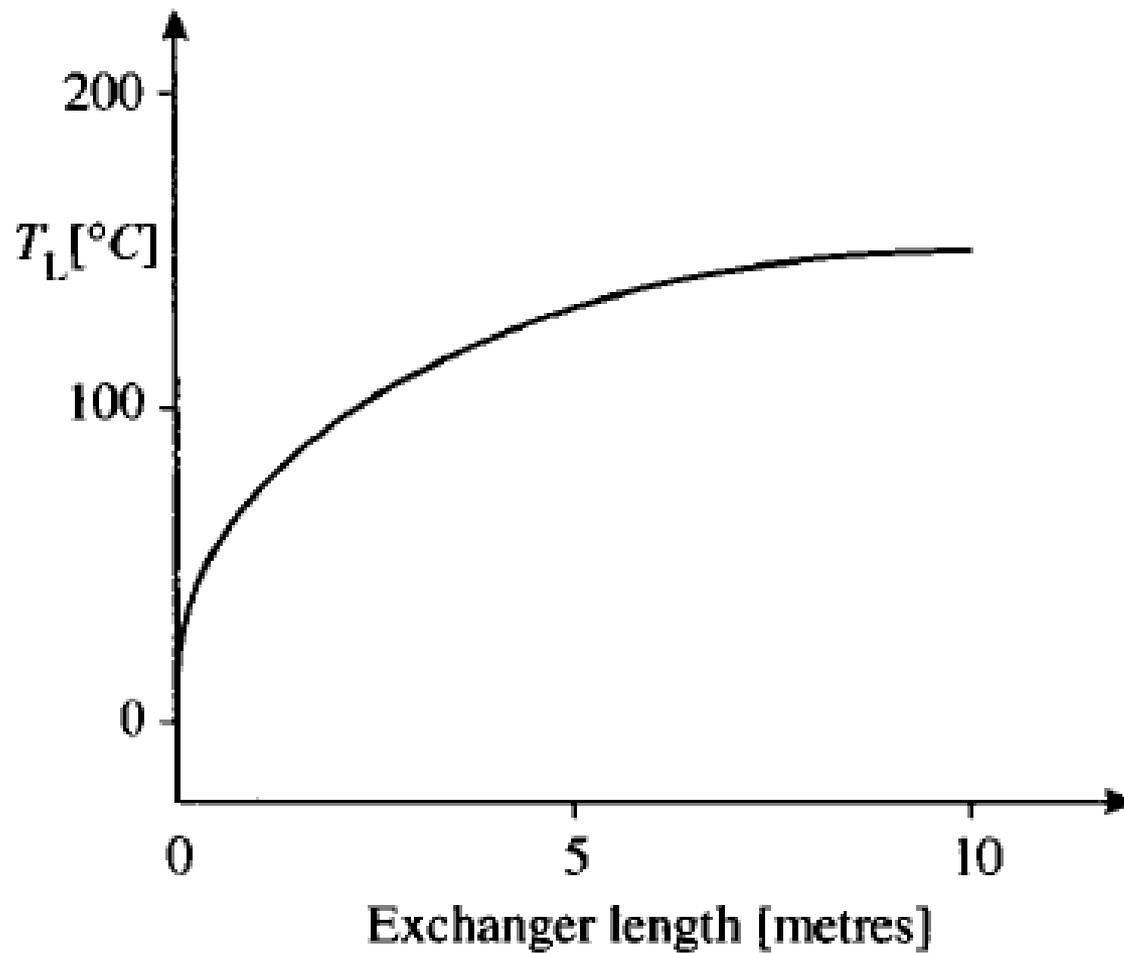
Steady-state temperature profile

EXAMPLE [(Modelling of a pollutant in a river)

Process system

- Here, we are concerned about a **pollutant discharged to a river and its subsequent concentration as it flows downstream**.

- The Figure below shows the geometry of the situation, showing the cross section of the river and the representative slice over which the conservation balances can be performed. Note that the axial distance is the co-ordinate length z.
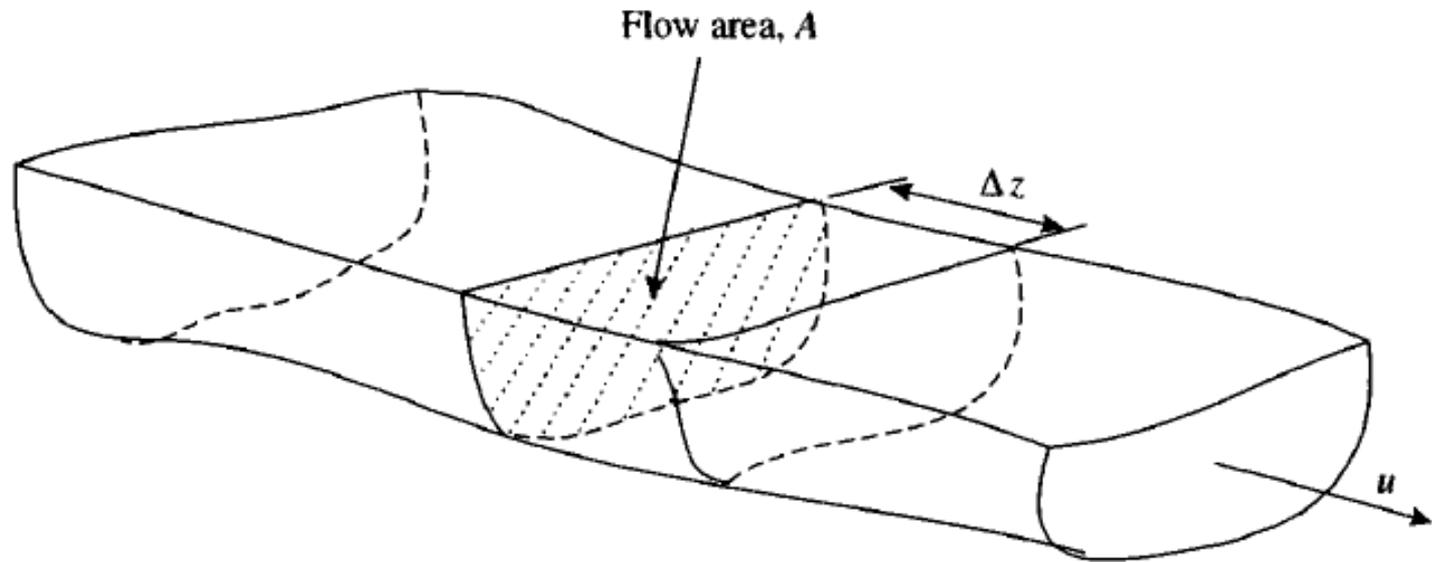
Pollutant dispersion in a river

Modelling goal

- To describe the distribution of the pollutant in the river.

Assumptions

- A 1 . The river has a constant cross-sectional area and the material is **ideally mixed over the cross section**.
- *A2. The pollutant **disappears via a first-order reaction**.*
- *A3. **Axial dispersion** is present.*
- *A4. No **radial dispersion**.*
- A5 . **River flow** is constant.
- *A6. The river water is considered **isothermal**.*
- *A7. **No pollution** is in the river in the beginning of the process.*

- **Balance volumes**

- A single distributed parameter volume encapsulating the whole river.

- **Model equations**

  Variables

  $$0 \le x \le L, \quad t \ge 0, \quad c(x, t),$$

- where x is the spatial coordinate in axial direction, L the length of the river, t the time, and c the pollutant concentration.

- *Component mass balance*

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial z} + D\frac{\partial^2 c}{\partial z^2} - kc,$$

with

c concentration $[\text{kg/m}^3]$

A flow area $[\text{m}^2]$

u flow velocity $[\text{m/s}]$

D dispersion coefficient $[\text{m}^2/\text{s}]$

k reaction rate $[\text{s}^{-1}]$

- **Initial and boundary conditions**

$$c(x, 0) = 0, \quad c(0, t) = C_A^{(i)},$$

where $C_A^{(i)}$ is the inlet concentration of the pollutant.

Normalization of the equations

- We can take the governing equation and define some non-dimensional groups as follows:

$$\theta = \frac{tu}{L}; \quad Pe = \frac{uL}{D}; \quad Z = \frac{z}{L}; \quad C = \frac{c}{c_0}; \quad K = \frac{kL}{u}$$

- and rearrange to get

$$\frac{\partial C}{\partial \theta} = -\frac{\partial C}{\partial Z} + \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - KC,$$

LUMPED PARAMETER MODELS FOR REPRESENTING DPSs

- Lumping of process models of DPS is a widely used technique **to transform the set of partial differential equations in the model into a set of ordinary differential equations**.

- The lumped model is **a finite approximation** of the DPS model in the space co-ordinate directions whereas the time variable remains the only independent variable in a lumped model.

- Most often models of **originally DPS systems** developed for dynamic analysis, control or diagnostic purposes are lumped in space.

The conceptual steps in lumping a DPS system model are as follows:

- 1. Divide the distributed parameter balance volume of the process system into a **finite number of subvolumes.**

- 2. Lump each subvolume into a perfectly mixed subvolume (call it lump) with **the variables averaged**.

- 3. Describe convection in the original DPS system as in- and outflows of the connected set of neighbouring lumps using the appropriate direction.

- 4. Describe **diffusion affecting all the neighbouring lumps** as in- and outflows of neighbouring lumps.

- 5. Use the **same sources for the lumps** as for the original DPS model.

- 6. Develop the **balance equations for every lump**.

- 7. Set **boundary conditions at the lumps** which coincide with the overall boundaries of the process system.

- **EXAMPLE (Lumped model of the double-pipe heat exchanger**).

Process system

- Consider the simple double pipe heat exchanger where the liquid stream is being heated by condensing saturated steam. The system is the same as in previous Example.

- Additional Assumptions to the ones listed as 1-7.

  A8. The heat exchanger is described as a sequence of **three well mixed volumes**.

- **Balance volumes**

- We consider two lots of three balance volumes with equal holdups.

- **Model equations**

  Variables

$$\left(T_L^{(k)}(t), T_W^{(k)}(t), \quad k = 1, 2, 3 \right), \quad 0 \leq t,$$

where $T_L^{(k)}(t)$ and $T_W^{(k)}(t)$ is the liquid and the wall temperature in the kth tank pair respectively and t is the time.

- *Energy balances for the liquid*

$$\frac{dT_L^{(k)}}{dt} = 3u\left(T_L^{(k-1)} - T_L^{(k)}\right) + \frac{1}{\tau_L}\left(T_w^{(k)} - T_L^{(k)}\right),$$

$$k = 1, 2, 3, \quad T_L^{(0)}(t) = T_L^{(i)}(t).$$

$T_L^{(i)}$ is the inlet fluid temperature to the whole reactor.

- *Energy balances for the wall*

$$\frac{dT_w^{(k)}}{dt} = \frac{1}{\tau_{sw}}\left(T_s - T_w^{(k)}\right) - \frac{1}{\tau_{wL}}\left(T_w^{(k)} - T_L^{(k)}\right), \quad k = 1, 2, 3.$$

- **Initial conditions**

$$T_L^{(k)}(0) = f_1^{(k)}, \quad k = 1, 2, 3,$$

$$T_w^{(k)}(0) = f_2^{(k)}, \quad k = 1, 2, 3$$

where the values of $f_1^{(k)}$, $k = 1, 2, 3$ and $f_2^{(k)}$, $k = 1, 2, 3$ are taken from the functions f_1 and f_2 at the appropriate spatial locations z_k, $k = 1, 2, 3$.