1. Introduction
to
Process System Engineering

Introduction

- **System Engineering** is the definition, design, development, production, and maintenance of functional, reliable, and trustworthy systems within cost and time constraints.

Other Definitions of SE

- **Structure**: SE is management technology to assist clients thru the formulation, analysis, and interpretation of the impacts of proposed policies, controls, or complete systems upon the need perspectives, institution perspectives, and value of stakeholders to issue under consideration.

- **Function**: SE is an appropriate combination of the methods and tools of systems engineering, made possible thru use of a suitable methodology and systems management procedures, in a useful process-oriented setting that is appropriate for the resolution of real-world problems, often of large scale and scope

- **Purpose:** **The purpose of SE is info and knowledge organization that will assist clients who desire to define, develop, and deploy total systems to achieve a high standard of overall quality, integrity, and integration as related to performance, trustworthiness, reliability, availability and maintainability of the resulting system.**

"The whole is more than the sum of its parts." Aristotle, 384 BC – 322 BC

- **SE is focused on the system as a whole– it emphasizes its total operation:**
  - **Looks at the system from the outside as well as the inside**
  - **Interactions with other systems and the environment**
  - **Concerned with not only engineering design but also external factors**

- SE is an **interdisciplinary approach** and means for enabling the realization and deployment of successful systems.

- It can be viewed as the **application of engineering techniques to the engineering of systems**, as well as the application of a systems approach to engineering efforts.

- SE **integrates other disciplines** and specialty groups **into a team effort**, forming a structured development process that proceeds from concept to production to operation and disposal.

- SE considers both **the business and the technical needs of all customers**, with the goal of providing a quality product that meets the user needs.

Process Systems Engineering (PSE)

- **Process Systems Engineering (PSE)** covers the activities involved in the engineering of systems with **physical, chemical, and/or biological processing** operations.

- The engineering of processing systems is as old as **the onset of the industrial revolution**, but the term PSE was only coined about 50 years ago at the outset of the modern era of **computer-aided engineering**.

- In recent years, PSE has expanded significantly **beyond its original scope,** the continuous and batch chemical processes and their associated process engineering problems.

- Today, it encompass **the creative design, operation, and control of biological systems, complex networks of chemical reactions, free or guided self-assembly processes, micro- and nano-scale processes, energy systems based on renewables**, and global **supply chains of fuels** and chemicals that involve environmental and life cycle issues.

Process modeling in PSE

- A model is **an imitation of reality** and a mathematical model is **a particular form of representation**.

- In the process of model building we are **translating our real world problem into an equivalent mathematical problem** which we solve and then attempt to interpret.

- We do this to gain insight into the original real world situation or **to use the model for control, optimization or possibly safety studies**.

- In the process engineering area the models we deal with are **fundamentally mathematical in nature**. They attempt to capture, in the form of equations, certain **characteristics of a system for a specific use of that model**.

- In building a model, we require that certain characteristics of the actual system be represented by the model.
- Those characteristics could include:
  - the correct **response direction of the outputs** as the inputs change;
  - **Valid structure** which correctly represents **the connection** between the inputs, outputs and internal variables;
  - the correct short and/or long term **behavior of the model**.

Modeling Steps

Reality to Mathematics (Step I)

- Here we have to deal with the task **of translating the real problem to one represented in mathematical terms**. Some of the key issues which have to be dealt with here are:
    - What do we understand about the **real world problem**?
    - What is **the intended use** of the mathematical model?
    - What **governing phenomena or mechanisms** are there in the system?
    - What **form of model** is required?
    - How should the model be **structured and documented?**
    - **How accurate** does the model have to be?
    - What data on the system are available and what is the **quality and accuracy** of the data?
    - What are the **system inputs, states, outputs and disturbances**?

Mathematical Solution (Step 2)

- Having generated some mathematical description of the real world system, it is then necessary **to solve this for the unknown value of the variables** representing that system.
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- Key issues here are:

  - **What variables** must be chosen in the model to satisfy the **degrees of freedom**?

  - Is the model solvable

-What **numerical (or analytic) solution technique** should be used?

- Can the structure of the problem be exploited **to improve the solution speed or robustnes**s?

- What **form of representation** should be used to display the results (2D graphs,3D visualization)?

- **How sensitive** will the solution output be to variations in the system parameters or inputs?

Interpreting the Model Outputs (Step 3)

- Here we need to have procedures and tests to check whether our model has been **correctly implemented** and then ask whether it imitates the real world to a sufficient accuracy to do the intended job. Key issues include:

- How is **the model implementation** to be verified?

- What type of **model validation** is appropriate and feasible for the problem? Is the resultant model identifiable?

- What needs to be **changed, added or deleted** in the model as a result of the validation?

- What **level of simplification** is justified?

-What **data quality and quantity** is necessary for validation and parameter estimates?

- What **level of model validation** is necessary?

- Should it be **static or dynamic**?

- What **level of accuracy** is appropriate?

- What system parameters**, inputs or disturbances**, need to be known accurately to ensure model predictive quality?

Using the Results in the Real World (Step 4)

- Here we are faced with the implementation of the model or its results back into the real world problem we originally addressed. Some issues that arise are:

  - Do I need to reduce the **model complexity**?

  - How can **model updating** be done and what data are needed to do it?
  - **Who will actually use** the results and in what form should they appear?
  - How is the model to be maintained?
  - What **level of documentation** is necessary?

Model Application Areas

Application area	Model use and aim
Process design	Feasibility analysis of novel designs Technical, economic, environmental assessment Effects of process parameter changes on performance Optimization using structural and parametric changes Analysing process interactions Waste minimization in design
Process control	Examining regulatory control strategies Analysing dynamics for setpoint changes or disturbances Optimal control strategies for batch operations Optimal control for multi-product operations Optimal startup and shutdown policies

Application area	Model use and aim
Trouble-shooting	Identifying likely causes for quality problems Identifying likely causes for process deviations
Process safety	Detection of hazardous operating regimes Estimation of accidental release events Estimation of effects from release scenarios (fire etc.)
Operator training	Startup and shutdown for normal operations Emergency response training Routine operations training
Environmental impact	Quantifying emission rates for a specific design Dispersion predictions for air and water releases Characterizing social and economic impact Estimating acute accident effects (fire, explosion)

MODEL CLASSIFICATION

- We can devise several ways of classifying models. Each **leads to a variety of model characteristics** which have an impact on the solution techniques as well as the potential **application areas where they can be used**.

- Some model types are inappropriate in certain circumstances, such as a steady-state model for batch reactor start-up analysis.

- The following Table gives an overview of **model types, their basic characteristics and the final form of the models**.

Type of model	Criterion of classification
Mechanistic	Based on mechanisms/underlying phenomena
Empirical	Based on input-output data, trials or experiments
Stochastic	Contains model elements that are probabilistic in nature
Deterministic	Based on cause-effect analysis
Lumped parameter	Dependent variables not a function of spatial position
Distributed parameter	Dependent variables are a function of spatial position
Linear	Superposition principle applies
Nonlinear	Superposition principle does not apply
Continuous	Dependent variables defined over continuous space-time
Discrete	Only defined for discrete values of time and/or space
Hybrid	Containing continuous and discrete behaviour

- **Mechanistic models** are also referred to **phenomenological models** because of their basic derivation from system phenomena or mechanisms such as mass, heat and momentum transfer.
- Many common models in process engineering applications are derived from a knowledge of the underlying mechanisms.
- However, **most mechanistic models also contain empirical parts** such as rate expressions or heat transfer relations.
- Mechanistic models often appear in design and optimization applications.
- They can be termed **"white box" models** since the mechanisms are evident in the model description.

- **Empirical models** are the result of **experiment and observation**, usually not relying on the knowledge of the basic principles and mechanisms which are present in the system being studied.

- They employ essentially **equation fitting** where the parameters have little or no physical meaning.

- Empirical models are widely used **where the actual underlying phenomena are not known or understood well**.

- These models are often termed **"black box" models**, reflecting the fact that little is known about the real mechanisms of the process.

- The most common form of model used in process engineering is **a combination of mechanistic and empirical parts** and hence is termed "grey box".

- **Stochastic models** arise when the description may contain elements which have **natural random variations** typically described **by probability distributions**.

- This characteristic is often associated with phenomena which are not describable in terms of cause and effect but rather by probabilities or likelihoods.

- **Deterministic models** are the final type of models characterized by clear **cause-effect relationships**.

- In most cases in process engineering the resultant model has elements from several of these model classes.

- Thus ,we can have a mechanistic model with some stochastic parts to it.

- A very common occurrence is a mechanistic model which includes empirical aspects such as **reaction rate expressions or heat transfer relationships**.

Equation form of Process Models

- We can also consider the types of equations which result from such models when we consider steady state and dynamic situations. These are shown in the next Table.

- The forms can involve **linear algebraic equations** (LAEs), **nonlinear algebraic equations** (NLAEs), **ordinary differential equations (ODEs), elliptic partial differential equations (EPDEs)** and **parabolic partial differential equations (PPDEs).**

- Each of the equation forms requires special techniques for solution.

Types of model	Equation Type	
	Steady State Problem	**Dynamic Problem**
Deterministic	Nonlinear algebraic	ODEs/PDEs
Stochastic	Algebraic equations	Stochastic ODEs or difference equations
Lumped Parameter	Algebraic equations	ODEs
Distributed parameter	EPDES	PPDEs
Linear	Linear algebraic equations	Linear ODEs
Non linear	Non-linear algebraic equations	Non-linear ODEs
continuous	Algebraic equations	ODEs
Discrete	Difference equations	Difference equations

Characteristics of the System Volumes

- When we develop models, it is necessary to **define regions in the system where we apply conservation principles** and basic physical and chemical laws in order to derive the mathematical description. These are the balance volumes.

- A basic classification relates to the nature of the material in those volumes. Where there are **both temporal and spatial variations in the properties of interest**, such as concentration or temperature, we call these systems "**distributed**".

- However, when there are no spatial variations and the material is homogeneous, we have a "**lumped**" system.

- The complexity of distributed parameter systems can be significant both in terms of the resulting model description and the required solution techniques. Lumped parameter models generally lead to simpler equation systems which are easier to solve.

- When we consider system modeling, there are many situations where discrete events occur, such as **turning on a pump** or **shutting a valve**.

- These lead to discontinuous behavior in the system either at a known time or at a particular level of one of the states such as temperature or concentration. These are called "time" or "state" events.

- A model which has both characteristics is termed a hybrid system. These are very common in process systems modeling.

- Not only do we need to consider the classification of the models that are used in PSE applications but it is also helpful to look at some characteristics of those models.

MODEL CHARACTERISTICS

- Here we consider some of the key characteristics which might affect our modeling and analysis.

- Models **can be developed in hierarchies**, where we can have several models for different tasks or models with varying complexity in terms of their structure and application area.
- Models exist **with relative precision**, which affect how and where we can use them.
- Models cause us **to think about our system** and force us to consider the key issues.
- Models can help direct **further experiments and in-depth investigations.**

- Models are **developed at a cost in terms of money and effort**. These need to be considered in any application.

- Models are **always imperfect**. It was once said , a well-known statistician, "**All models are wrong, some are useful"!**

- Models invariably **require parameter estimation** of constants within the model such as kinetic rate constants, heat transfer and mass transfer coefficients.

- Models can often be **transferred from one discipline to another**.

- Models should **display simplest form** to achieve the desired modeling goal.

- Models **should be identifiable** in terms of their internal parameters.

- Models may often **need simplification,** or model order reduction to become useful tools.

- Models may be difficult or impossible to **adequately validate**.

A BRIEF HISTORICAL REVIEW OF MODELLING IN PSE

- As a distinct discipline, PSE is **a child of the broader field of systems engineering** as applied to processing operations.

- As such, its appearance as a recognized discipline dates back to the **middle of the twentieth century.**

- In this section, we trace briefly the history of model building, analysis and model use in the field of PSE.

The Industrial Revolution

- It was **the industrial revolution** which gave the need to systematic approaches for the analysis of processing and manufacturing operations.

- Those processes were no longer simple tasks but **became increasingly complex in nature** as **the demand for commodity products increased**.

- In particular, the early chemical developments of the late eighteenth century spurred on by the Franco-British wars led to industrial scale processes for the manufacture of **gun powder, sulphuric acid, alkali** as well as food products such as **sugar from sugar beet.**

- In these developments the French and the British competed in the development of new production processes, aided by the introduction of steam power in the early 1800s which greatly **increased potential production capacity.**

- In dealing with these new processes, it was necessary for the engineer to bring to bear on **the problem techniques derived from many of the physical sciences and engineering disciplines.**

- These analysis techniques quickly recognized the **complex interacting behavior of many activities**. These ranged from manufacturing processes to communication systems.

- The complexities varied enormously but the approaches took on a "**systems**" view of the problem which gave due regard to the components in **the process, the inputs, outputs of the system and the complex interactions** which could occur due to the connected nature of the process.

- Random use of systems engineering as a sub-discipline of industrial engineering in the nineteenth and twentieth centuries **found application in many of the industrial processes developed in both Europe and the United States**.

- This also coincided **with the emergence of chemical engineering** as a distinct discipline **at the end of the nineteenth century** and **the development of the unit operations concept** which would dominate the view of chemical engineers for most of the twentieth century.

- There was a growing **realization that significant benefits would be gained** in the overall economics and performance of processes **when a systems approach** was adopted. This covered the design, control and operation of the process.

- In order to achieve this goal, there was **a growing trend to reduce complex behaviour to simple mathematical forms for easier process design**—hence the **use of mathematical models**.
- The early handbooks of chemical engineering, were dominated by the equipment aspects with **simple models for steam, fluid flow and mechanical behaviour** of equipment.
- They were mainly descriptive in content, emphasizing the role of the chemical engineer as one who ensured:

  ... ***Completeness of reactions, fewness of repairs and economy of hand labour.***

- Little existed in the area of **process modelling aimed at reactor and separation systems**.

- In the period from **1900 to the mid-1920s** there was a fast growing body of literature on more **detailed analysis of unit operations**, which saw an increased reliance on mathematical modelling.

- **Heat exchange, drying, evaporation, centrifugation, solids processing and separation technologies such as distillation** were subject to the application of mass and energy balances for model development.

The Mid-twentieth Century

- After the end of the Second World War there was a growing interest in the application of systems engineering **approaches to industrial processes, especially in the chemical industry**.
- The **mid-1950s saw many developments in the application of mathematical modeling to process engineering unit operations**, especially for the understanding and prediction of the behavior of individual units.
- This was especially true in the area of **chemical reactor analysis**. Many prominent engineers, mathematicians and scientists were involved.
- It was a period of applying rigorous mathematical analysis to process systems which up until that time had not been analyzed in such detail.
- However, the efforts were mainly **restricted to specific unit operations and failed to address the process as a "system**".
- This interest in mathematical analysis coincided with the early development and growing availability of computers. **This has been a major driving force in modeling ever since.**

- One of the earliest monographs on PSE appeared in 1961 as a result of work within the Monsanto Chemical Company in the USA. This was authored by T.J. Williams who wrote:

  ... **Systems engineering has a significant contribution to make to the practice and development of chemical engineering. The crossing of barriers between chemical engineering and other engineering disciplines and the use of advanced mathematics to study fundamental process mechanisms cannot help but be fruitful**.

- He continued,

  ... the **use of computers and the development of mathematical process simulation techniques may result in completely new methods and approaches** which will justify themselves by economic and technological improvements.

The Modern Era

- The vision of T.J. Williams was not met within the 1960s but tremendous strides were made in the area of process modeling and simulation.

- The seminal work on transport phenomena by **Bird *et al.*** *in 1960 gave further drive to the* mathematical modeling of process systems through the use of fundamental principles of conservation of mass, energy and momentum.

- It has remained the pre-eminent book on this subject for over 40 years.

- The same period saw **the emergence of numerous digital computer simulators for both steady state and dynamic simulation**. These were both industrially and academically developed tools. Many of the systems were forerunners of the current class of steady state and dynamic simulation packages.

- They were systems **which incorporated packaged models for many unit operations with little ability for the user to model specific process operations** not covered by the simulation system.

- The numerical routines **were crude by today's standards** but simply reflected the stage of development reached by numerical mathematics of the time.

- Efficiency and robustness of **solution were often poor** and diagnostics as to what had happened were virtually non-existent. Some things have not changed!

- **The development of mini-computers in the 1970s** and the emergence of **UNIX based computers followed by the personal computer (PC)** in the early 1980s **gave a boost to the development of modeling and simulation tools.**

- It became a reality that every engineer could have a simulation tool on the desk which could **address a wide range of steady state and dynamic simulation problems.**

- This development was also reflected in the process industries where equipment vendors were beginning to supply **sophisticated distributed control systems (DCSs)** based on mini- and microcomputers.

- These often incorporated simulation systems based on simple block representations of the process or in some cases incorporated real time higher level computing languages **such as FORTRAN or BASIC**.

- The systems were **capable of incorporating large scale real time optimization** and supervisory functions

- Accompanying the development of the process simulators was an attempt to provide computer aided modelling frameworks for the generation of process models **based on the application of fundamental conservation principles** related to mass, energy and momentum.

- These have been **almost exclusively in the academic domain with a slowly growing penetration into the industrial arena**.

- What continues to be of concern is **the lack of comprehensive and reliable tools for process modeling** and the almost exclusive slant towards the petrochemical industries of most commercial simulation systems.

- The effective and efficient development of mathematical models for new and non-traditional processes **still remains the biggest hurdle to the exploitation of those models** in PSE.

- This is especially the case in the non-petrochemical sector such as **minerals processing, food, agricultural products, pharmaceuticals, wastewater and the integrated proces**s and manufacturing industries where large scale discrete-continuous operations are providing the current challenge.