

Lecture#1 Introduction to Modeling in Chemical Engineering

Goal

This lecture introduces students to the fundamental concepts of modeling as a core analytical tool in chemical engineering. The main objective is to develop an understanding of how mathematical models are constructed, applied, and validated to describe chemical and physical processes, predict system behavior, and support design, optimization, and safety in chemical industries.

Introduction. Modeling in chemical engineering is a critical tool used to predict and optimize the behavior of chemical processes. This lecture will provide an introduction to modeling, focusing on the principles behind it, and explore several real-world applications in chemical engineering, illustrating how models can be employed to solve problems in various industries.

What is Modeling?

In simple terms, a model is a mathematical representation of a system or process. In chemical engineering, modeling is used to describe and simulate the behavior of chemical processes, reactors, and systems. This enables engineers to predict how systems will behave under different conditions, optimize processes, and troubleshoot issues.

Why is Modeling Important?

- Prediction and Optimization: Models allow engineers to predict the behavior of systems without needing to experiment with real systems, saving time and resources.
- Process Understanding: Through modeling, engineers can gain deeper insights into complex systems, leading to better process control.
- Design and Scale-up: Modeling plays a vital role in designing new processes and scaling them up from laboratory to industrial scale.
- Safety: By simulating hazardous conditions, models can help prevent dangerous situations in chemical plants.

Types of Models in Chemical Engineering

Empirical Models: Based on experimental data. These models often fit curves or equations to observed data and are less focused on physical laws.

Mechanistic Models: Based on fundamental principles such as mass, energy, and momentum conservation. These models are more general and predictive.

Stochastic Models: These account for randomness and uncertainties in the process, useful in systems where variability is significant.

Applications of Modeling in Chemical Engineering

Process Design and Simulation

Modeling plays a key role in the design of new processes and the optimization of existing ones.

- Process Simulators: Software like Aspen Plus, HYSYS, and PRO/II are used to simulate chemical processes. These tools use thermodynamic and kinetic models to predict the behavior of unit operations such as reactors, distillation columns, heat exchangers, and pumps.

- Design of Distillation Columns: For separating mixtures, engineers use models to predict the number of theoretical stages, reflux ratios, and energy consumption.

- Reactor Design: Models help predict conversion, selectivity, and yield in reactors, optimizing reaction conditions and catalyst design.

Example: In the oil refining industry, models are used to optimize the cracking process, which breaks down large hydrocarbons into smaller ones like gasoline and diesel. By simulating different operating conditions, refineries can maximize yield and minimize energy use.

Environmental Engineering

Chemical engineering modeling is essential in environmental engineering for pollution control, waste treatment, and resource management.

- Air Pollution Control: Models are used to predict the dispersion of pollutants in the atmosphere. For example, Gaussian plume models estimate the

concentration of pollutants emitted from industrial sources based on wind speed, emission rates, and atmospheric stability.

- Wastewater Treatment: Modeling helps in designing biological reactors used for treating wastewater. These models simulate microbial activity, enabling engineers to optimize the removal of contaminants such as nitrogen and phosphorus.

Example: Modeling the dispersion of sulfur dioxide (SO_2) emissions from power plants allows engineers to evaluate the effectiveness of scrubbers and other control technologies.

Energy and Sustainability

Energy generation and sustainability are growing areas where chemical engineers apply modeling.

- Energy Systems: Modeling is used to optimize chemical processes in energy production, such as natural gas reforming, coal gasification, or renewable energy production (e.g., hydrogen production from electrolysis).

- Sustainability Assessments: Life-cycle assessment (LCA) models evaluate the environmental impacts of products or processes over their entire life cycle—from raw material extraction to disposal.

Example: In carbon capture and sequestration, models simulate the absorption of CO_2 into solvents and predict the energy required for regeneration of the solvent, helping to optimize CCS systems.

Challenges and Limitations in Chemical Engineering Modeling

While modeling is a powerful tool, it is not without challenges:

- Data Requirements: Models often require a large amount of data, which may not always be available or accurate.

- Simplifications and Assumptions: Engineers often make assumptions (e.g., ideal behavior or steady-state conditions) to simplify complex systems, which can lead to errors.

- Uncertainty and Sensitivity: Models may be sensitive to uncertainties in input parameters, and small changes in conditions can result in significant deviations in predictions.
- Computational Complexity: Some models, especially those involving detailed mechanistic processes or multiphase flows, can be computationally intensive and require sophisticated software and hardware.

Conclusion

Modeling in chemical engineering is an essential tool for process design, optimization, and innovation across various industries. From environmental protection to pharmaceuticals, and energy systems to polymer manufacturing, modeling allows chemical engineers to predict the behavior of complex systems, make informed decisions, and ultimately design more efficient, safer, and sustainable processes. However, it is important to understand the limitations and challenges associated with modeling, such as data accuracy and computational complexity, in order to use it effectively.

Learning Outcomes

By the end of this lecture, students will be able to:

- 1. Define the concept of modeling and explain its importance and role in chemical engineering (related to LO 1, ID 1.1).*
- 2. Identify and classify different types of models used in chemical engineering — empirical, mechanistic, and stochastic (related to LO 1, ID 1.1).*
- 3. Explain the capabilities and limitations of modern modeling tools (e.g., COMSOL Multiphysics, Aspen Plus) (related to LO 1, ID 1.2).*
- 4. Describe major applications of modeling in process design, optimization, environmental engineering, and sustainable energy systems (related to LO 1, ID 1.1 and 1.2).*
- 5. Recognize typical challenges and limitations in modeling practice, including data uncertainty, model assumptions, and computational complexity (related to LO 1, ID 1.2).*

Questions and Self-study Assignments

1. Define the term “model” and explain how it is used in chemical engineering.
2. Compare and contrast empirical, mechanistic, and stochastic models, giving one example of each.
3. Discuss at least three advantages of modeling over direct experimentation.
4. Identify and describe two real-world applications of modeling in process design or environmental protection.
5. Explain what limitations or assumptions can affect the accuracy of a chemical process model.
6. Read one recent (within the last 3 years) journal article describing the use of modeling in chemical or electrochemical process design, and summarize:
 - the type of model used;
 - main objectives;
 - conclusions regarding optimization or sustainability.

References

1. Finlayson B.A. Introduction to Chemical Engineering Computing. Second Edition. - John Wiley & Sons, 2012. ISBN 9781118309599, DOI: 10.1002/9781118309599
2. Pryor R.W. Multiphysics Modeling Using COMSOL5 and MATLAB. - Mercury Learning and Information, 2015. – 700 p. ISBN 1938549988