LECTURE 01

Introduction to Modeling in Chemical Engineering

Department of Analytical, Colloidal Chemistry and Technology of Rare Elements

Modeling of chemico-technological processes | 6B07102 Chemical Engineering

Khaisa Avchukir, PhD, Acting Associate Professor

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Purpose and expected learning outcomes

Purpose: develop physically grounded models that connect measurable chemical-engineering behavior to governing equations and reliable predictions.

EXPLAIN

Identify governing phenomena and state assumptions.

CALCULATE

Apply equations using consistent physical units.

COMPARE

Evaluate alternative model formulations.

INTERPRET

Read simulated curves and measured responses.

EVALUATE

Test limitations, uncertainty and validity.

APPLY

Propose a reproducible modeling workflow.

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From physical system to engineering decisions

01 Define system

Boundaries, outputs

02 Formulate physics

Balances and kinetics

03 Specify parameters

Units and assumptions

04 Solve equations

Analytical or numerical

05 Validate outputs

Experiment and errors

06 Optimize process

Design and control

Industrial relevance: reactors • separations • electrolysis • energy storage • environmental treatment

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What is a process model?

A model maps operating conditions and parameters to measurable process outputs.

$$y = f(u, \theta, t)$$

MODEL CONDITIONS u: inputs; θ: parameters; y: outputs. Define a control volume before writing equations.

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What Is a Mathematical Model?

A mathematical model is a simplified mathematical representation of a real-world system or process.
It describes relationships between input variables, internal process variables, and output variables using mathematical equations.
For example, consider a chemical reactor in which a reactant A is converted into product B:
A → B
The concentration of reactant A decreases with time as the reaction proceeds.
For a first-order reaction, the rate of reaction is proportional to the concentration of reactant A:

$$-r_A = kC_A$$

where:

- r_A is the rate of consumption of reactant A.
- k is the reaction rate constant.
- C_A is the concentration of reactant A.

For a batch reactor with constant volume: $dC_A/dt = -kC_A$

The solution is: $C_A = C_{A,0} \exp(-kt)$

where $C_{A,0}$ is the initial concentration and t is time.
This equation represents a mathematical model of the reaction process.
It allows engineers to predict reactant concentration at any given time without performing an experiment for every possible time point.

Why Is Modeling Important in Chemical Engineering?

Mathematical modeling plays a central role in modern chemical engineering because it provides opportunities to study and improve processes before implementing them in industrial facilities.

1. Process Understanding

Models help explain the relationships between process variables and identify the mechanisms controlling process behavior.

For example, a reactor model can show how reaction temperature influences the reaction rate and product yield.

2. Process Design

Models are used to determine equipment dimensions, operating conditions, and process configurations.

For example, engineers can estimate the required reactor volume to achieve a specified conversion.

3. Process Optimization

Modeling makes it possible to identify operating conditions that maximize product yield, minimize energy consumption, or reduce production costs.

4. Process Safety

Models can predict potentially dangerous conditions, including excessive temperatures, pressure increases, and unstable reaction behavior.

5. Cost and Time Reduction

Computer simulations reduce the need for numerous expensive laboratory and pilot-scale experiments.

6. Environmental Protection

Models help predict pollutant formation, wastewater treatment efficiency, emissions, and the environmental impact of industrial processes.

Conservation as the modeling foundation

A species balance accounts for accumulation, flow, and reaction.

$$dN_i/dt = F_{i,in} - F_{i,out} + \int_V r_i \, dV$$

MODEL CONDITIONS N_i is amount (mol); F_i is molar flow (mol s^{-1}); r_i is net generation (mol m^{-3} s^{-1}).

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Classification of Models in Chemical Engineering

Chemical engineering models can be classified according to their physical nature, mathematical structure, and the approach used to describe a process.

1. Physical Models

Physical models are scaled or simplified physical representations of real industrial systems.

Examples include:

- Laboratory-scale reactors.
- Pilot-scale distillation columns.
- Scaled fluid-flow systems.
- Physical models of heat exchangers.

Physical modeling is particularly useful when complex flow patterns or equipment geometry cannot be adequately represented using simple analytical equations.

2. Mathematical Models

Mathematical models describe processes using equations, functions, and mathematical relationships.

Examples include:

- Differential equations describing reaction kinetics.
- Algebraic equations describing chemical equilibrium.
- Mass balance equations.
- Heat transfer equations.

3. Empirical Models

Empirical models are developed using experimental data and statistical relationships.

They do not necessarily describe the fundamental physical or chemical mechanisms of a process.

For example:

$$Y = a + bX$$

where: Y is the process response. X is an independent variable. a and b are regression coefficients.

Empirical models are useful when sufficient experimental data are available and the objective is to predict process behavior within the investigated experimental range.

4. Mechanistic Models

Mechanistic models are based on fundamental scientific principles and describe the physical and chemical mechanisms occurring within a system.

They are generally developed using:

- Conservation of mass.
- Conservation of energy.
- Conservation of momentum.
- Chemical reaction kinetics.
- Thermodynamic relationships.
- Transport phenomena.

For example, a mechanistic model of a chemical reactor may combine reaction kinetics with material and energy balances.

5. Hybrid Models

Hybrid models combine mechanistic principles with empirical or data-driven approaches.

For example, a reactor model may use:

- A mass balance based on conservation laws.
- A neural network to predict a complex reaction rate.
- Experimental data to estimate unknown parameters.

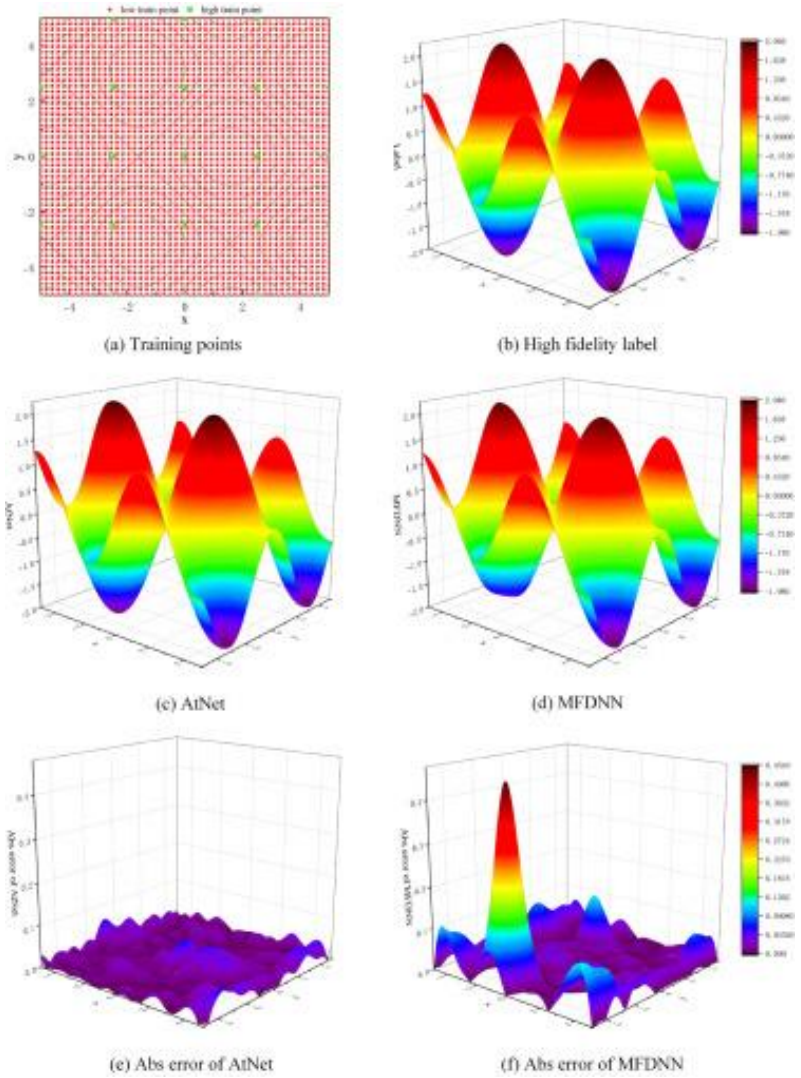
Hybrid modeling is increasingly important in modern chemical engineering because it combines physical understanding with the predictive capabilities of artificial intelligence and machine learning.

Model classes and fidelity

Mechanistic, empirical and stochastic descriptions answer different questions.

$$y = f_{physics}(u, \theta) + \varepsilon$$

MODEL CONDITIONS ε represents measurement/model discrepancy; a stochastic term needs a specified distribution.



Fazhi Tang, Yubo Li, Jun Huang, Feng Liu, Multi-fidelity modeling method based on adaptive transfer learning, Information Fusion, Volume 120, 2025, 103045, ISSN 1566-2535,https://doi.org/10.1016/j.inffus.2025.103045.

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From process diagram to equations

Specify boundaries, state variables, initial conditions and constraints.

state $\dot{x} = f(x,u,\theta)$; output $y = g(x,u,\theta)$

MODEL CONDITIONS A steady-state model sets $\dot{x} = 0$; transient start-up requires initial $x(0)$.

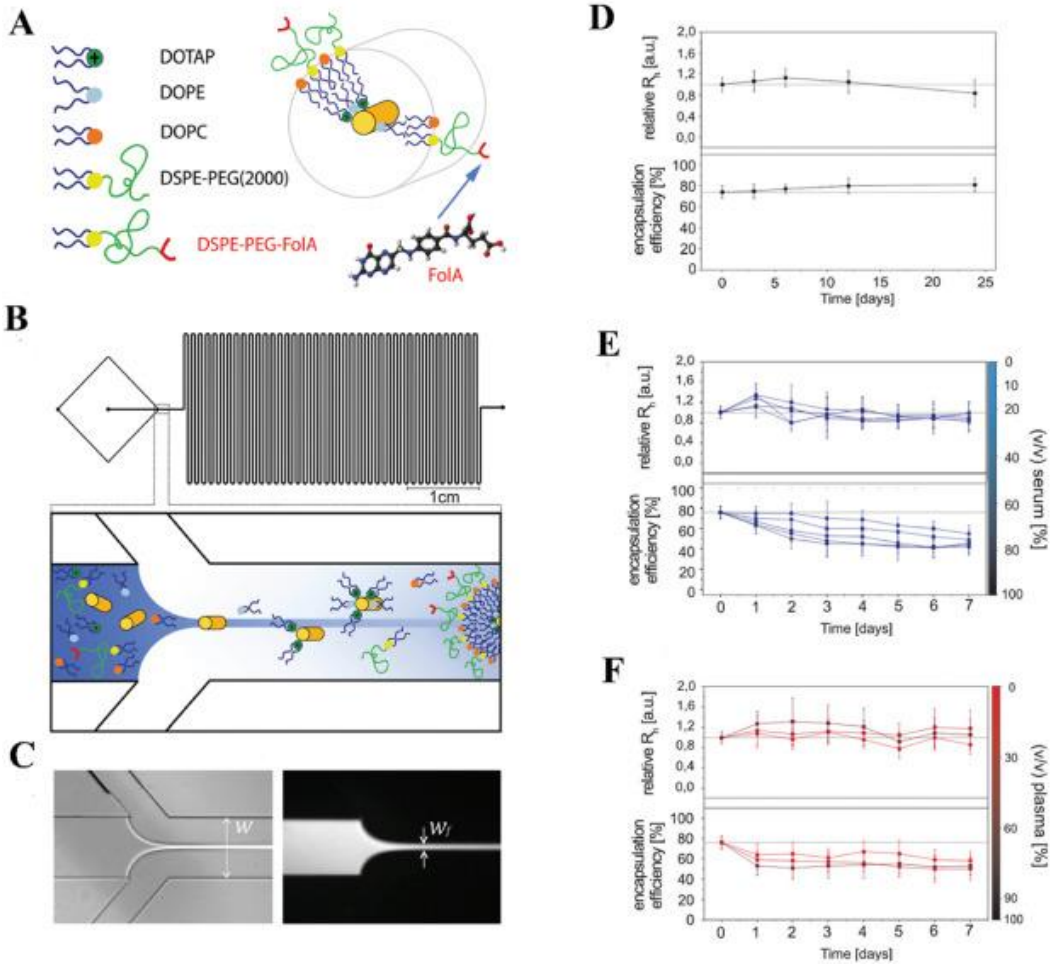
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Scale-up and sensitivity

Dimensionless groups help identify which physics remain important at larger scales.

Re = ρvL/μ; Pe = vL/D

MODEL CONDITIONS Re compares inertia with viscosity; Pe compares advection with diffusion.



https://doi.org/10.1016/j.mtchem.2026.103863

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Validation, uncertainty and safety

Fit parameters using training data, then evaluate predictions independently.

$$RMSE = \sqrt{[\Sigma(y_{obs} - y_{pred})^2/N]}$$

MODEL CONDITIONS Use hold-out operating conditions and check physical constraints.

ENGINEERING INTERPRETATION Scenario simulations support hazard analysis but cannot replace experiments.

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Components of a Mathematical Model

A complete mathematical model generally contains several interconnected elements.

1. Model Variables

Variables describe the state and behavior of the system.

They can be divided into:

Independent variables: time, position, temperature, or other variables used to define the conditions of the system.

Dependent variables: concentrations, pressure, temperature, conversion, and reaction rate.

Input variables: quantities supplied to the process, such as feed flow rate and feed concentration.

Output variables: measurable results, such as product concentration, conversion, and production rate.

2 **Model Parameters**

Parameters are quantities that characterize the process and are usually determined experimentally or obtained from scientific literature.

Examples: Reaction rate constant; Activation energy; Heat transfer coefficient.

3. Initial Conditions

Initial conditions specify the state of the system at the beginning of a dynamic process.

For example:

$C_A(0) = C_{A,0}$

4. Boundary Conditions

Boundary conditions specify the values or behavior of variables at the boundaries of a spatial domain.

For example, the temperature at the inlet of a tubular reactor may be specified as:

$T(0,t) = T_{in}$

Conclusions: a verified model is a useful model

PHYSICS

Identify dominant conservation and transport laws.

EQUATIONS

State variables, signs, units and assumptions.

PARAMETERS

Determine measurable coefficients and uncertainty.

NUMERICS

Check stability, convergence and physical balances.

EXPERIMENT

Validate predictions with independent observations.

APPLICATION

Use models for design, control and optimization.

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Conclusion

Mathematical modeling is one of the fundamental tools of modern chemical engineering.
It provides a systematic approach to understanding, predicting, designing, and optimizing chemical processes.
The development of a mathematical model requires:

- Understanding the physical and chemical mechanisms of a process.
- Applying fundamental conservation laws.
- Identifying variables and parameters.
- Formulating governing equations.
- Solving mathematical equations.
- Calibrating, verifying, and validating the model.

The integration of mathematical modeling with computational methods, artificial intelligence, and experimental research is transforming modern chemical engineering and supporting the development of more efficient, sustainable, and intelligent industrial processes.

Homework: calculations, interpretation and research

1. THEORY Explain the assumptions behind “$y = f(u, \theta, t)$” and identify when they fail.

2. CALCULATION For $C_0 = 2.0\ \text{mol m}^{-3}$, $k = 0.020\ \text{s}^{-1}$ and $t = 60$ s, calculate $C = C_0 \exp(-kt)$ and conversion.

3. DATA Simulated normalized outputs at $t = 0, 20, 40, 60$ s are 1.00, 0.67, 0.45, 0.30. Estimate a first-order rate constant.

4. CRITIQUE Explain how transport limitations or nonideal mixing could invalidate a simple rate model.

5. RESEARCH Design a two-condition validation experiment for introduction to modeling in chemical engineering; report measured variables, units and uncertainty.

Constants when needed: $F = 96485\ \text{C mol}^{-1}$; $R = 8.314\ \text{J mol}^{-1}\ \text{K}^{-1}$; $T = 298.15$ K.

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Recommended Literature

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