Scale-Up of Chemical Engineering Process
Chapter 4: Overview on Mathematical Modeling in Chemical Engineering

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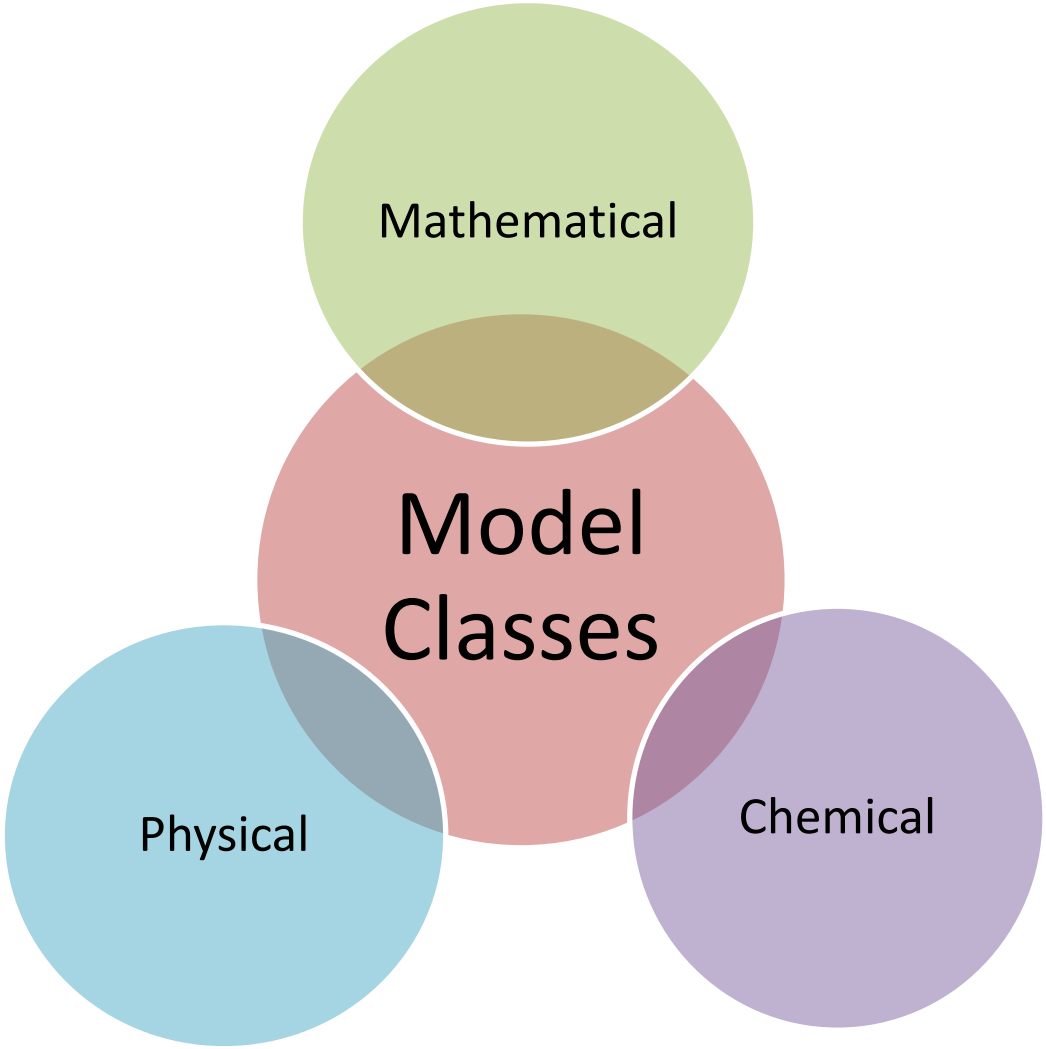
Model

- Definition:
  - The approximate representation of a process, mechanism or phenomenon.
  - This representation may or may not rely on concrete material support.



Models are prerequisite for:

- design and scale-up;
- process control;
- optimization;
- mechanistic understanding;
- evaluation/planning of experiments;
- trouble shooting and diagnostics;
- determining quantities that cannot be measured directly;
- simulation instead of costly experiments in the development lab;
- feasibility studies to determine potential before building prototype equipment or devices.

Why modeling?

- The need to represent and condense the data
- Separation of essential from accessory, clarification, identification etc
- Forecasting the behavior of the system
- beyond the domain investigated
- Establishment of scale-up rules for designing industrial plants
- Development of optimal control system for a given operation
- Training in running production units

Why need mathematical models?

- Engineering is more easily conducted by means of NUMBERS
- Everything needs to be QUANTIFIED
- Engineer must be able to TRANSLATE any problems into NUMBERS, by which they make sizing of process equipment

Translation into math expression

- Verbal statement:

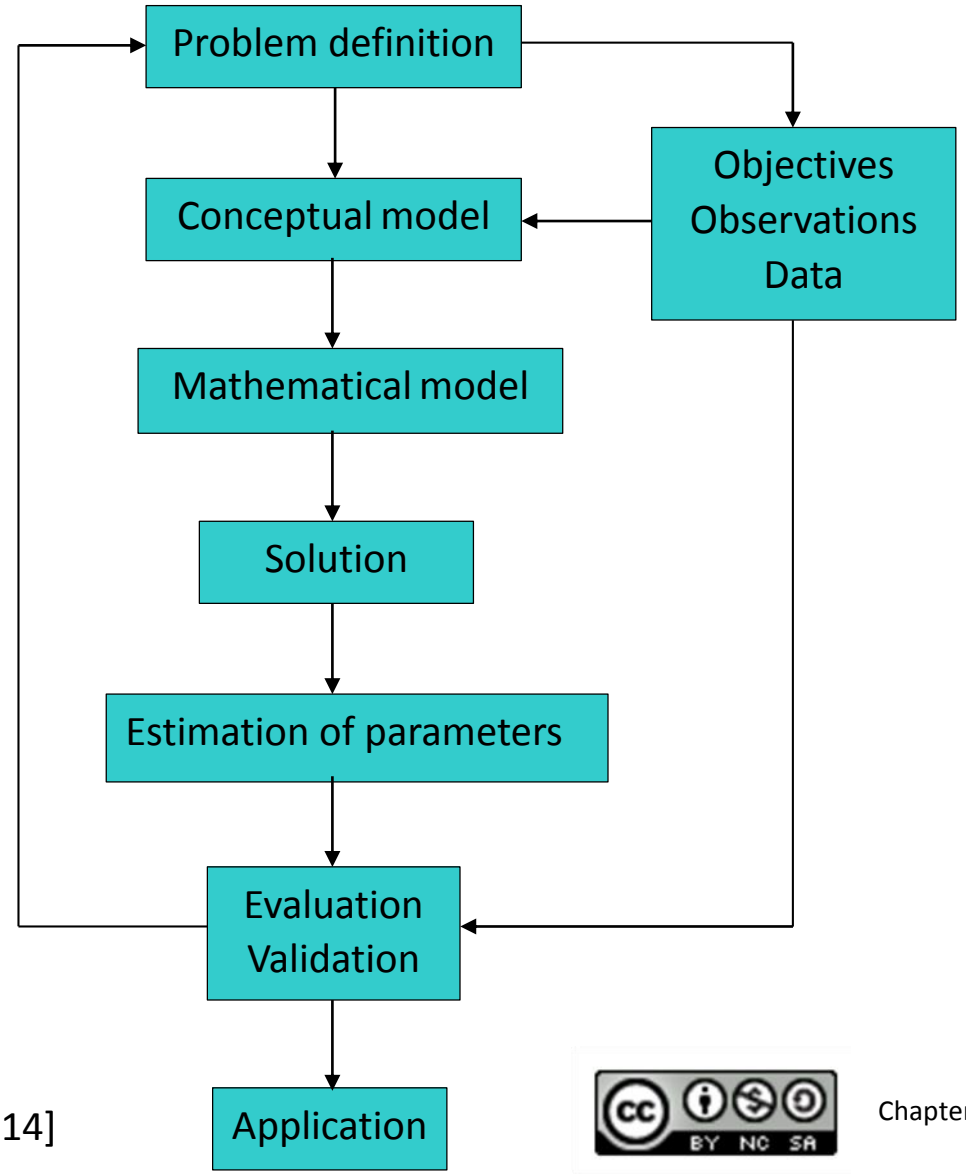
The concentration of reactant A is decreasing with increasing time

- Mathematical expression:

$$C_A = C_{Ao} - k_1 t^3 - k_2 t^2 - k_3 t$$

or $$-\frac{dC_A}{dt} = k_1 C_A$$ or $$-\frac{dCA}{dt} = k_2 C_A{}^n$$

Steps in model development



[Source: Rasmuson et al. 2014]

Categories of mathematical models

- Empirical model
- Deterministic model
- Stochastic model

Empirical models

$$C_A = C_{Ao} - k_1 t^3 - k_2 t^2 - k_3 t$$

- Any mathematical expressions with some adjustable parameters
- No particular theoretical background
- Example:

  polynomials

Deterministic models

- Based on theoretically accepted laws
- Example:

  From kinetics:

$$-\frac{dC_A}{dt} = k_1 C_A$$

Stochastic models

- Take into account the uncertainty of the phenomenon
- Incorporating the concept of probability into deterministic model
- Example:

  in processes involving living organisms in which uncertainty need to be considered

Comparison

	Empirical	Deterministic	Stochastic
Difficulty	<	>	>>>
Accuracy	<	>>	>>>

Focus for undergraduate level

DETERMINISTIC MODELS

Author Information

Credit to the author:

Prof Ir Dr Badhrulhisham Abdul Aziz

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