

Scale-Up of Chemical Engineering Process

Chapter 4: Overview on Mathematical Modeling in Chemical Engineering

by

Nurul Sa'aadah Sulaiman

Faculty of Chemical and Natural Resources Engineering
saadah@ump.edu.my



Chapter 4 by Nurul Sa'aadah

Mathematical model

*mathematical expressions that represents
some phenomena*



Chapter 4 by Nurul Sa'adah

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:

$$C_A = C_{A0} - k_1 t^3 - k_2 t^2 - k_3 t$$

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



Chapter 4 by Nurul Sa'adah

Categories of mathematical models

- Empirical model
- Deterministic model
- Stochastic model



Chapter 4 by Nurul Sa'adah

Empirical models

$$C_A = C_{A0} - k_1 t^3 - k_2 t^2 - k_3 t$$

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



Deterministic models

- Based on **theoretically accepted laws**
- Example:

From kinetics:

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



Chapter 4 by Nurul Sa'adah

Stochastic models

- Take into account the uncertainty of the phenomenon
- Incorporating the concept of probability into deterministic model
- Example:
in processes involving living organisms



Comparison

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



Focus for undergraduate level

DETERMINISTIC MODELS



Chapter 4 by Nurul Sa'adah

Author Information

Credit to the author:

Prof Ir Dr Badhrulhisham Abdul Aziz



Chapter 4 by Nurul Sa'adah