Scale-Up of Chemical Engineering Process

Chapter 5: Mathematical Modeling Strategy in Chemical Engineering

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Principles in math modeling

- Think simple:

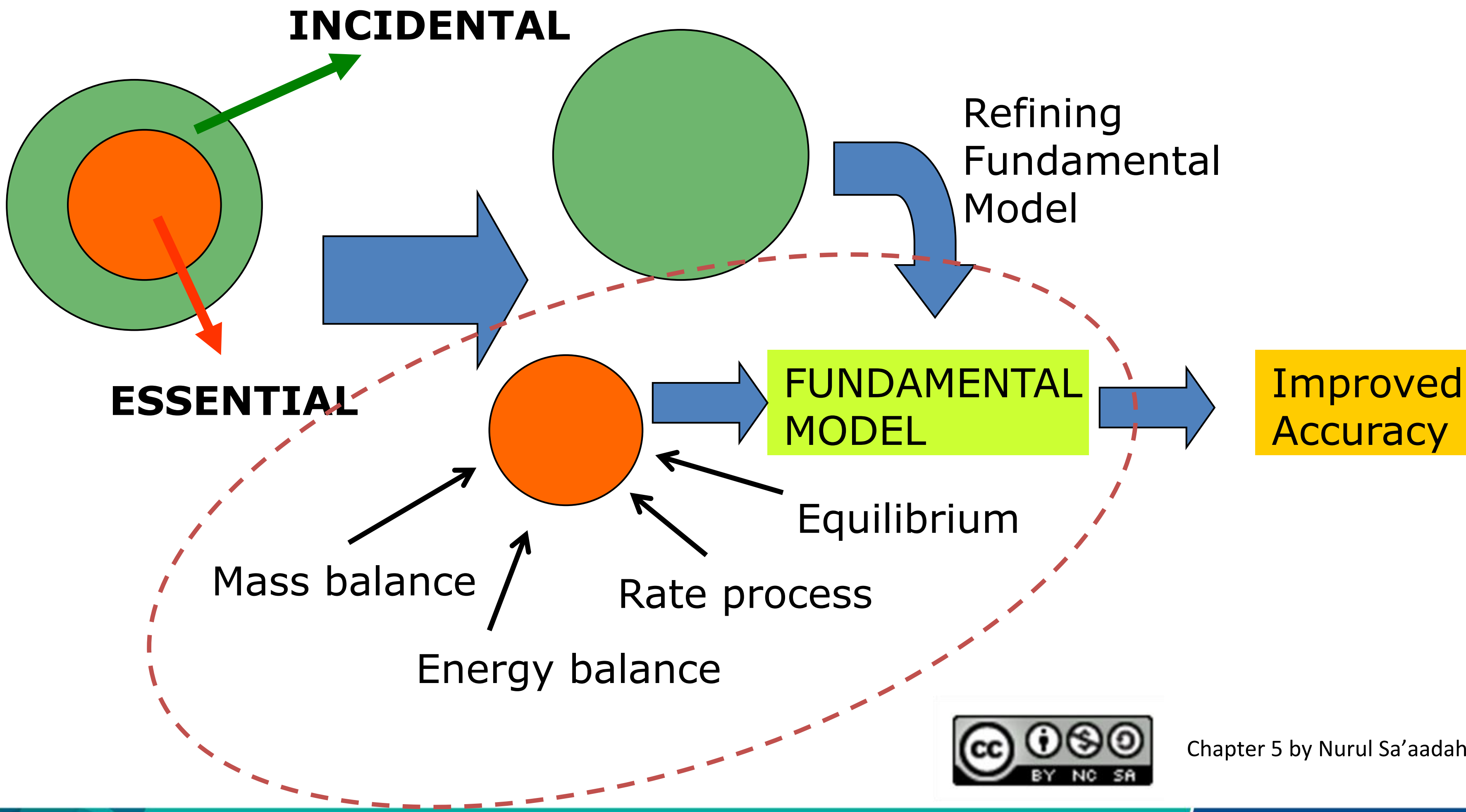
  -Separate the incidental from the essentials; focus on the essentials

  -Simplify general equation

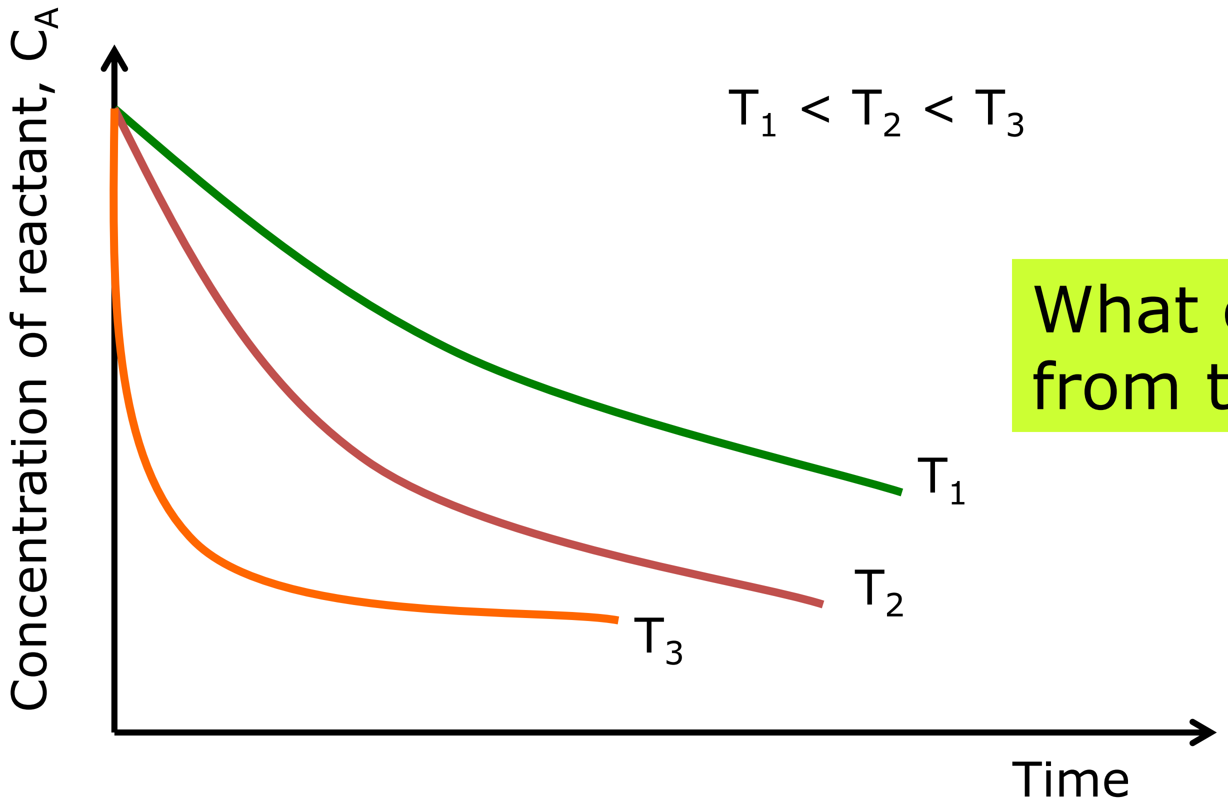
- Back to basic:

  -Mass balance, energy balance, rate processes, equilibrium

Principles in math modeling



Example: Batch Reactor Data



What can you infer from the data?

Data Observation

- Reactant depletion over time
- Different set of data for different temperature
- Reactant depletes more quickly at higher temperature

Which one essential and which one incidental?

Essential vs. incidental

- What essential:

  DEPEND ON YOUR MOST FUNDAMENTAL PURPOSE
- With respect to batch reaction data:

  your final goal is to design a reactor
- The size of reactor:

  depend on how fast the reaction is

  $\rightarrow$ the essential of the model is relation between C_A and time

  $\rightarrow$ temperature is incidental factor

Focus on the Essential

- How to correlate C_A and time?
- Back to basic: rate process for reaction is governed by reaction kinetics law
- In batch reactor (one of the possibilities):

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

Model's Variables and Constants

- Variable:
  Independent
  Dependent
- Constants:
  Adjustable parameters to fit the data on particular mathematical model

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

Example to find model constants

- Experimental data:

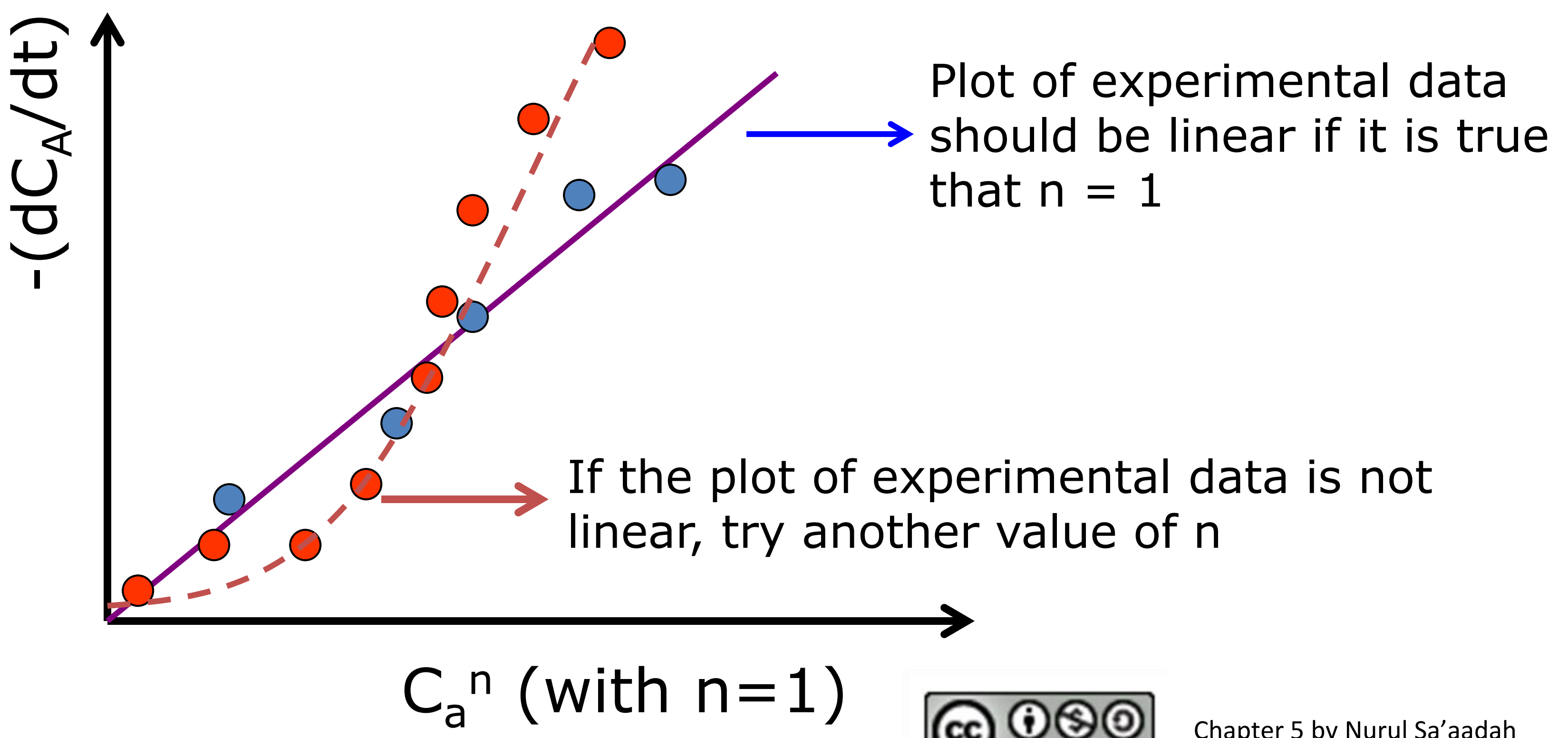
For T_1:

t	**C_A**	$(-dC_A/dt)$
t_1	C_{A1}	y_1
t_2	C_{A2}	y_2
.	.	.
.	.	.
t_n	C_{An}	y_3

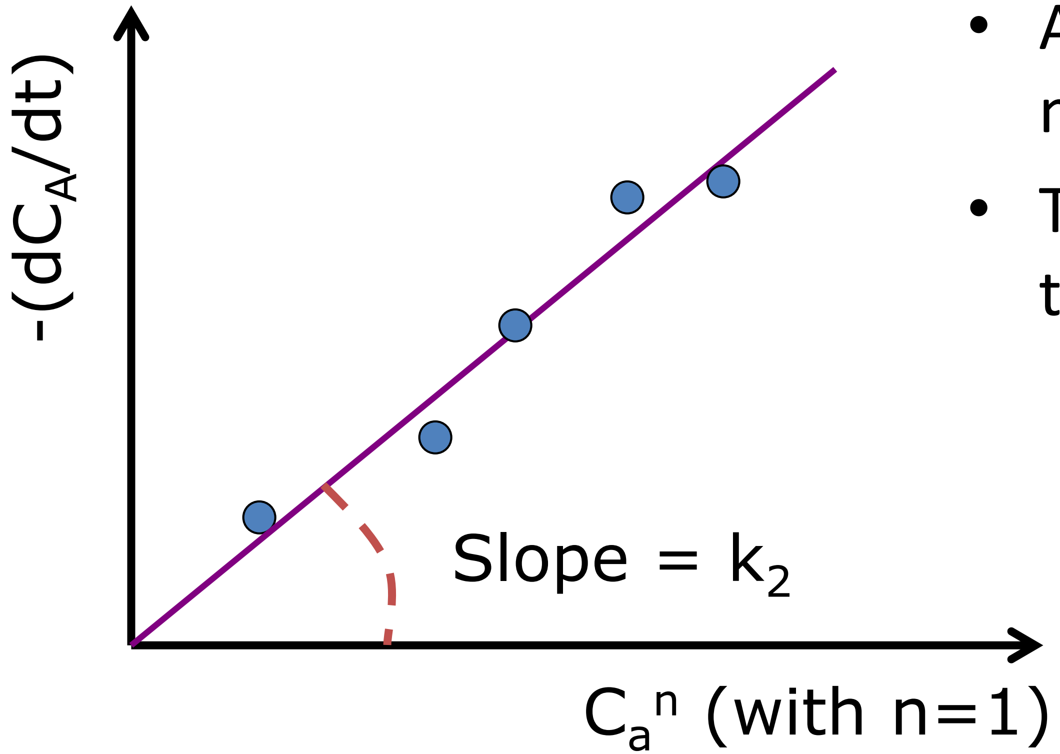
$$-\frac{dC_A}{dt} = k_2 C_A{}^n$$

Trial and Error Procedure

- Try n=1



Determination of k_2



- Assume it is correct that n = 1
- The value of k_2 is then the slope of the plot

Incorporating the Incidentals

- From the example, you may get 3 different values of k_2 for three different temperatures:

T	k_2
T_1	$(k_2)_1$
T_2	$(k_2)_2$
T_3	$(k_2)_3$

Correlating k_2 and T

Back to basic:

- use Arrhenius correlation;

$$k = A \exp(-E/R/T)$$

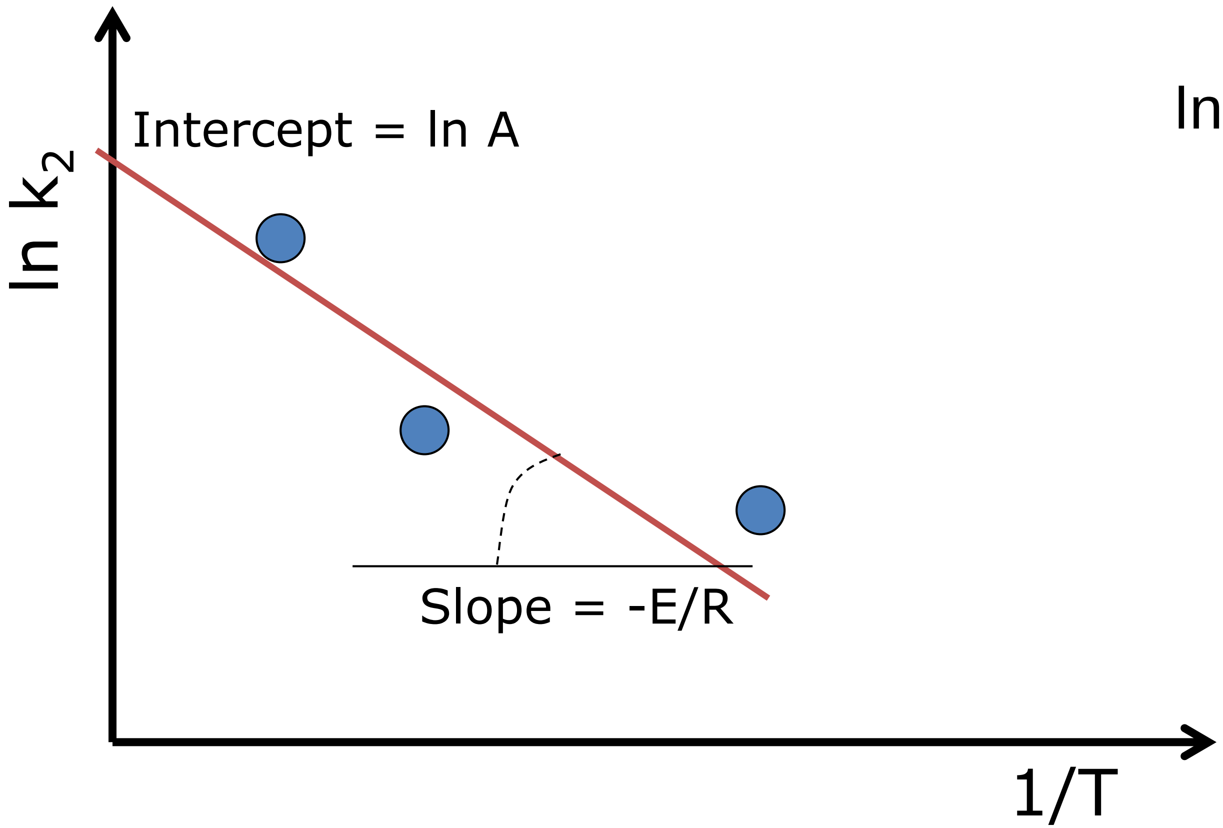
Correlating k_2 and T

$$k_2 = A \exp\left(-\frac{E}{RT}\right)$$

$$\ln k_2 = \ln A - \frac{E}{R}\left(\frac{1}{T}\right)$$

Plot of ln k_2 vs. (1/T)

Correlating k_2 and T



$$\ln k_2 = \ln A - \frac{E}{R}\left(\frac{1}{T}\right)$$

Complete model

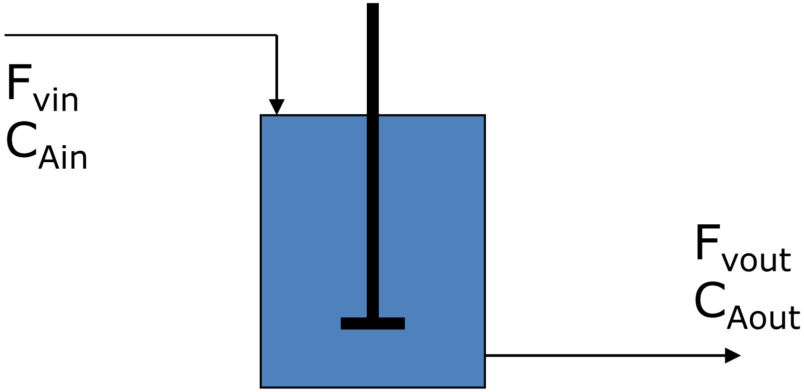
- Combining the essential and incidental, you get kinetic model:

$$(-r_A) = -\frac{dC_A}{dt} = A\exp\left(-\frac{E}{RT}\right)C_A$$

- You can predict the concentration of remaining A in the reactor at any time and temperature!

Utilizing kinetics model in CSTR design

- Back to basic: use mass balance (assuming isothermal reactor)



Rate of mass in + Rate of mass formed by reaction - Rate of mass reacted - Rate of mass out = Rate of accumulation

Steady-state CSTR modeling

Rate of mass in	+	Rate of mass formed by reaction	-	Rate of mass reacted	-	Rate of mass out	=	Rate of accumulation
$F_{vin}.C_{Ain}$	+	0	-	$(-r_A).V$	-	$F_{vout}.C_A$	=	0

$$V = \frac{F_{Vin}.C_{Ain} - F_{Vout}.C_{Aout}}{(-r_A)}$$

$$(-r_A) = A\exp\left(-\frac{E}{RT}\right)C_A$$

USEFUL FOR SCALE-UP

Other tools for scale up

- Correlations among dimensionless groups
- Empirical, but alright as long as you pick the correct dimensionless groups

Quantitative Approach in Scale-up (Mathematical Modeling)

Lab scale

Math modeling

Simulation

Pilot plant scale

Model improvement

Engineering design

Commercial scale

Important Tools for Scale-up

- Reliable correlations of dimensionless groups
- Reliable mathematical models
- Numerical methods to solve the models

Required Fundamentals

- Mass balance
- Energy balance
- Rate processes

  Physical: momentum transfer, mass transfer, heat transfer

  Chemical: reaction rate
- Equilibrium:

  Phase equilibrium

  Chemical equilibrium

Accuracy

- Highly accurate models: time/energy consuming, costly
- Moderately accurate models: quick, low cost
- For engineering purpose: does not need 100% (absolute) correct answers $\rightarrow$ we can do with 'careful estimation based on theoretical supports'

Author Information

Credit to the author:

Prof Ir Dr Badhrulhisham Abdul Aziz