CHN-323
Computer Applications in Chemical Engineering

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What is chemical engineering

- Chemical engineering simply deals with producing chemicals at large-scale
- A chemist found that A and B react to give C. To do so successfully, he first mixed A and B in a test tube by shaking and then used a burner to heat the mixture. In doing so, the chemical conversion happened. C is a precipitate that needs to be separated out. He used filter paper to separate the liquid and solids. The amount of C, he made is in grams.
- If C is to be produced in Tons, what should we do?

What is chemical engineering

Chemical Engineering

Biotechnology
Medical devices/diagnostics
genetic engineering
Pharmaceuticals

Food
Agriculture productivity
smart packaging
preservation

Environment
Catalytic converters
recycled materials
waste reduction

Materials
Polymers/plastics
ceramics
coatings

Energy
Petrochemicals
solar panels
fuel cells

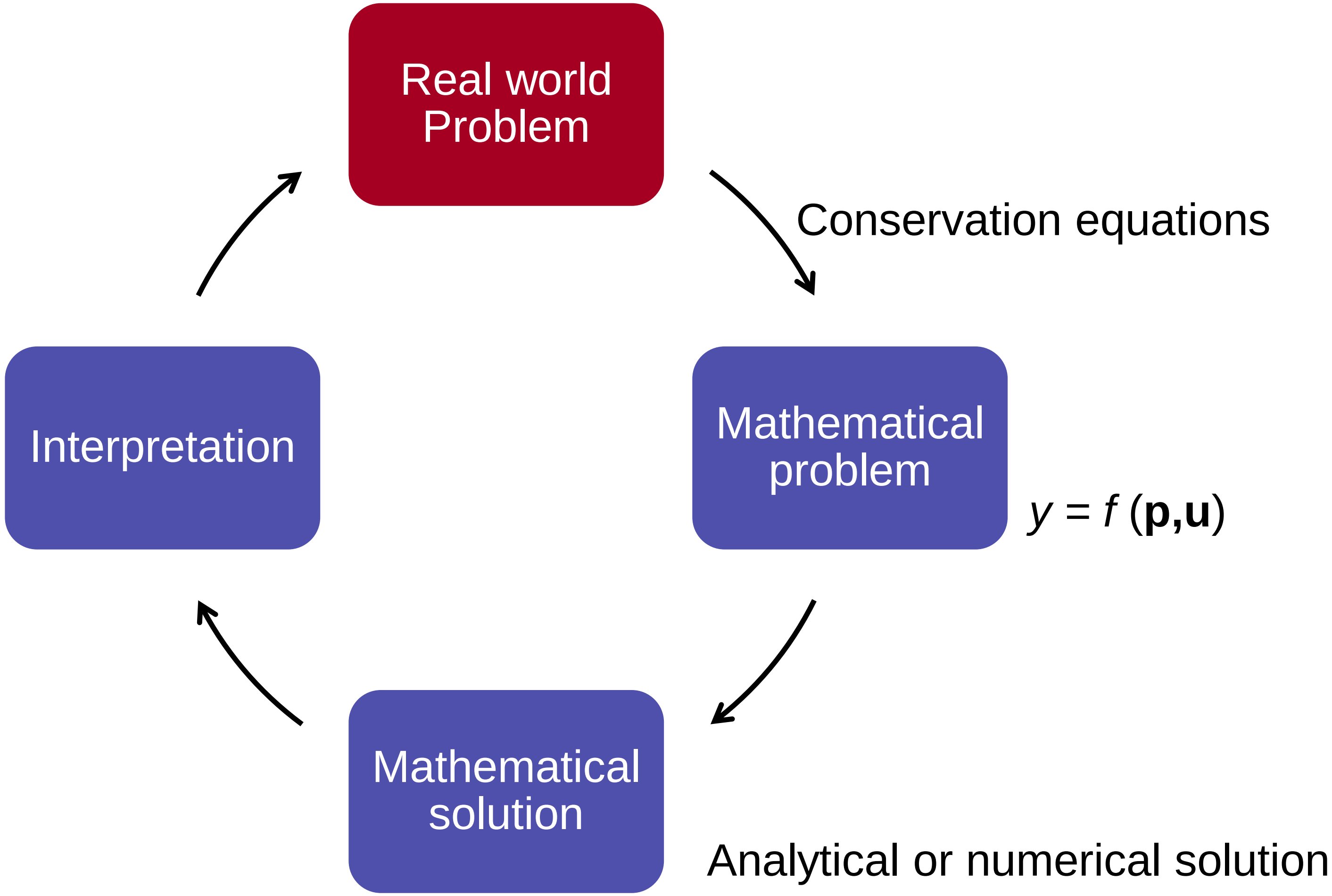
Information
Pentium – chip manufacture
semiconductors
optical fibers

Computer applications

- Why computers are required in chemical engineering?
- Engineers convert real-life problems into mathematical problems
- Mathematical problems means set of equations
  - Mathematical modeling: writing equations that describe system of interest for a specific purpose
- Not every equation can be solved with pen and paper (analytical solution)

Computer applications

- Computers can help us to solve the equations
- Numerical solution of equations: Simulation



Example 1

- *Can I calculate the boiling time for a soft-boiled egg, given its weight and initial temperature?*

- http://newton.ex.ac.uk/teaching/CDHW/egg/

- http://newton.ex.ac.uk/teaching/CDHW/egg/CW061201-1.pdf

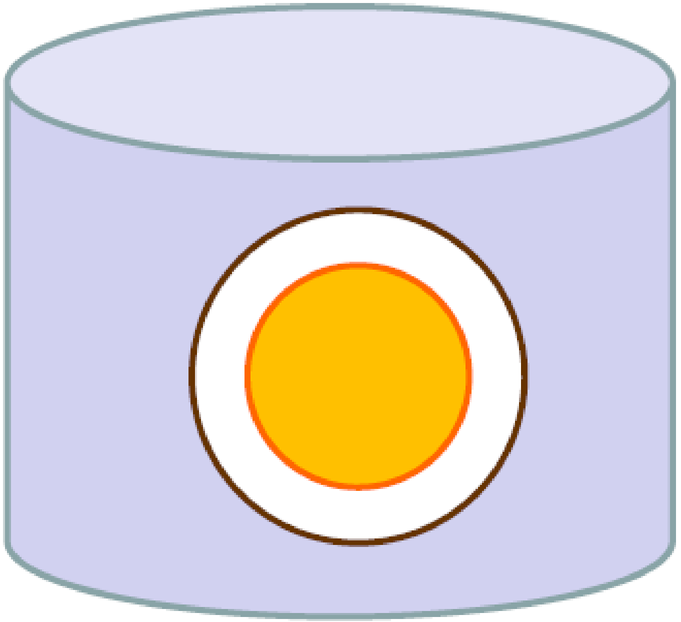
Boiling time of an egg

Real world problem

- Assumptions
  - Spherical egg
  - Egg is considered to be cooked when the T at boundary of the yolk reaches 63 ^{o}C

Boiling time of an egg

Real world problem $\xrightarrow{1}$ Mathematical problem



$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) = \frac{\tau_0 r^2}{a^2}\left(\frac{\partial T}{\partial t}\right)$$

http://newton.ex.ac.uk/teaching/CDHW/egg/CW061201-1.pdf

Boiling time of an egg

Real world problem $\xrightarrow{1}$ Mathematical problem

Mathematical problem $\xrightarrow{2}$ Mathematical solution

$$t_{\text{cooked}} = \frac{M^{2/3} c \rho^{1/3}}{K \pi^2 (4\pi/3)^{2/3}} \log_e \left[0.76 \times \frac{(T_{\text{egg}} - T_{\text{water}})}{(T_{\text{yolk}} - T_{\text{water}})} \right]$$

Boiling time of an egg

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) = \frac{\tau_0 r^2}{a^2}\left(\frac{\partial T}{\partial t}\right)$$

Real world problem

1

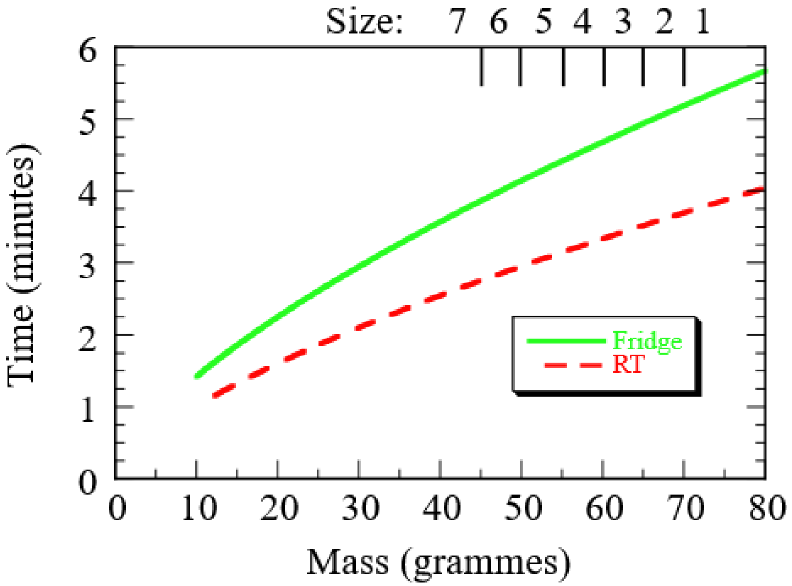
Mathematical problem

2

Mathematical solution

3

4



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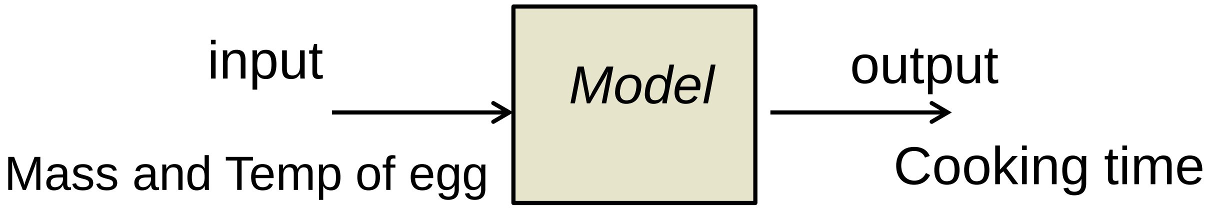
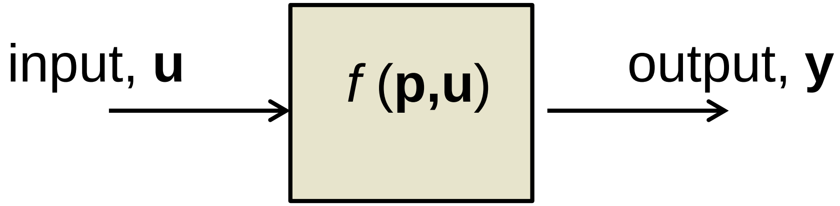
Theoretical modeling

- We just now completed a theoretical modeling problem
  - Physics-based modeling/Mechanistic modeling
  - Used theory/concept of conservation of energy to write the equation for temperature

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) = \frac{\tau_0 r^2}{a^2}\left(\frac{\partial T}{\partial t}\right)$$

  - Partial differential equation
  - Computers are required to simulate equations





Empirical modeling

- Observation-based modeling
  - You can conduct experiments for different eggs and temperatures, and measure the boiling times

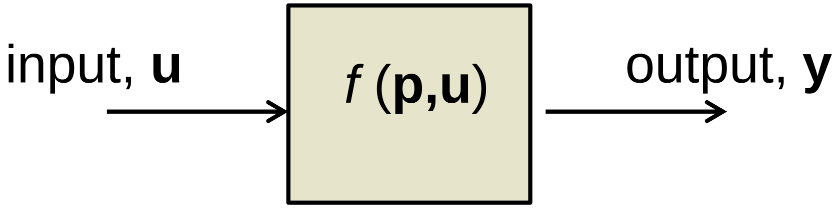
Can I calculate the boiling time for a soft-boiled egg, given its weight and initial temperature?

  - You will get some data
  - Data can be fitted to equations
  - Again, computers are needed

Observations

- Conduct experiments
- Collect data
- Data-fitting

Mass of egg (gm)	Temperature of egg (^oC)	Time to cook (measured) (mins)
80	4	6
80	21	4
60	4	4.75
60	21	3.25
40	4	3.5
40	21	2.5
20	4	2.25
20	21	1.6
10	4	1.4
10	21	1



Cooking time = *f* (mass of egg, temperature of egg)

Two modeling approaches: summary

Theoretical Modeling	Process Identification
First principles, white box (chemistry, physics, etc.)	Data driven modeling, black box, empirical
Requires sufficient knowledge about the process	Requires only the process output data in response to changes in input
Provides information about the internal state of the process	Provides information only about process input-output
Typically requires fewer measurements to estimate unknown model parameters	Requires extensive measurements as accuracy relies entirely on data

Usage of mathematical modeling

- Consider a chemical reaction between A and B.
  - The conversion might depend on several parameters, e.g., c_A, c_B, T, pH, shaking rpm.
  - Let us say, we have 5 values for each of the parameters.
  - You want to optimize the process conditions
  - 5^5=3125 number of expts required

Conversion = $f\,(c_A, c_B, T, pH, \text{shaking rpm})$

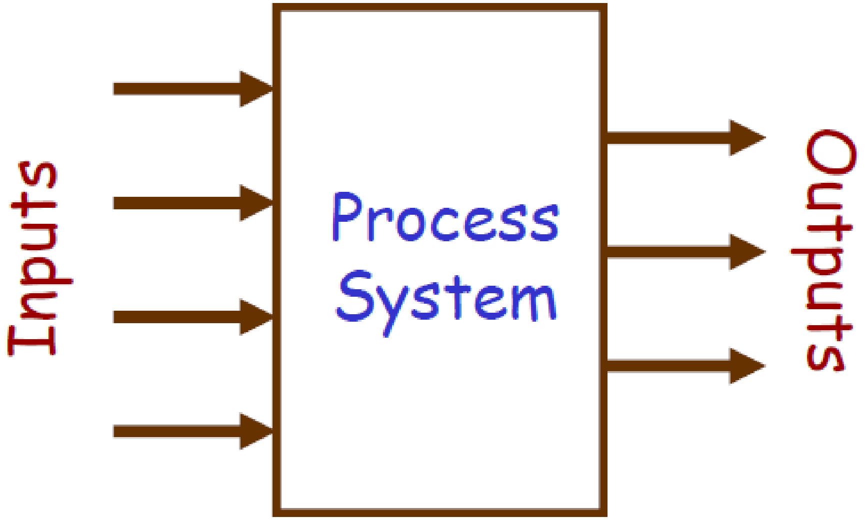
Usage of mathematical modeling

Prof. George Box once said

"All models are wrong. Some models are useful"

- In what ways, can a model be useful?
  - Process Design (known, ?, known)
  - Process Simulation (known, known, ?)
  - Control Design (?, known, known)
  - Process Optimization

  ....



Why this course?

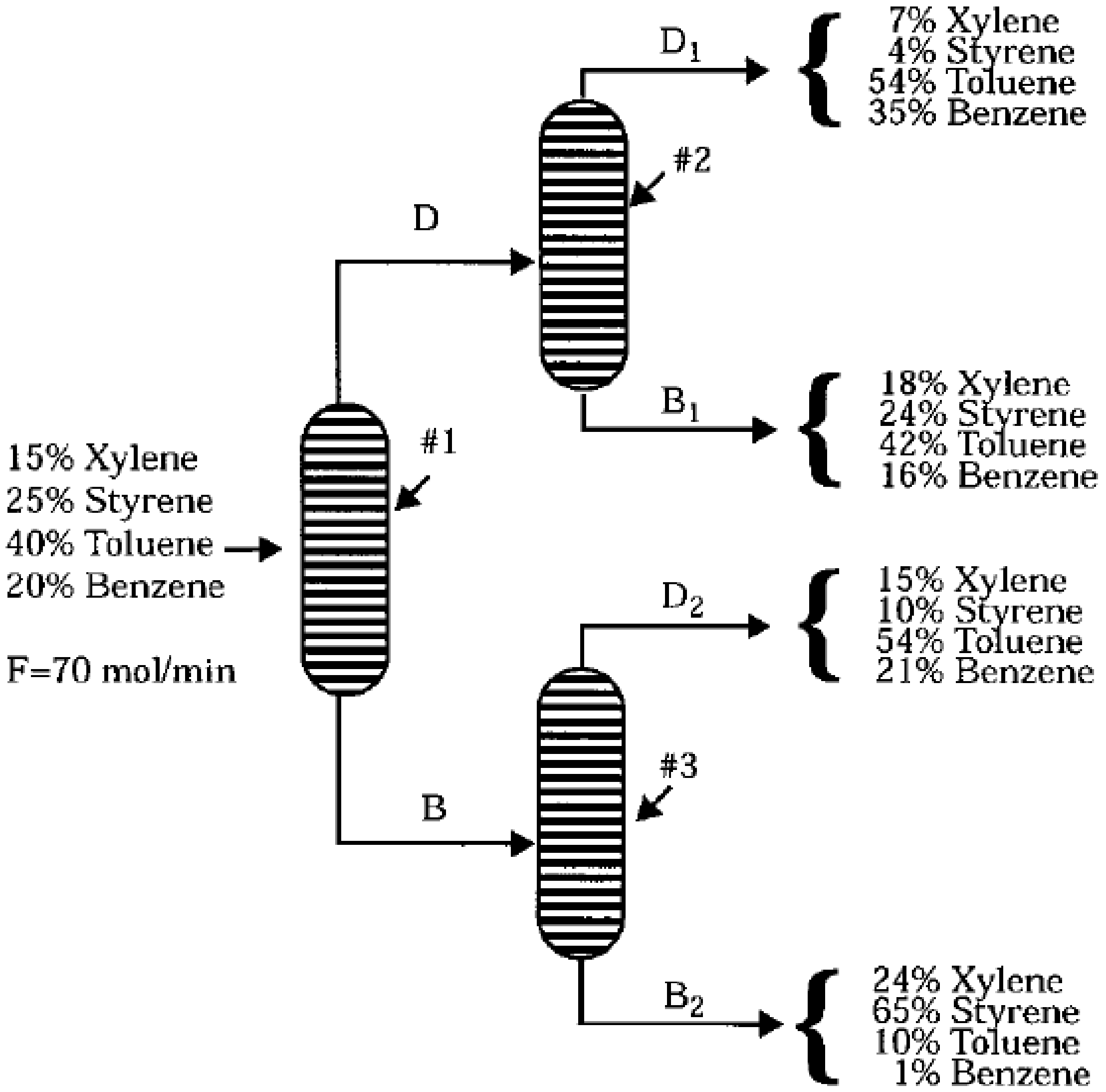
- Van der Waals equation of state

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT \qquad a = \frac{27}{64}\left(\frac{R^2T_c^2}{P_c}\right) \qquad b = \frac{RT_c}{8P_c}$$

- P (atm), V(L/gmol), R=0.08206 atm.L/(gmol. K)
- T_c=405.5 K, P_c=111.3 atm for ammonia

- Calculate the molar volume and compressibility factor for ammonia gas at a pressure of 56 atm and a temperature of 450 K.

Why this course?



$$\text{Xylene: } 0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15 \times 70$$

$$\text{Styrene: } 0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 0.25 \times 70$$

$$\text{Toluene: } 0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 0.40 \times 70$$

$$\text{Benzene: } 0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.20 \times 70$$

Why this course?

Table A.1 Vapor Pressure of Benzene (Perry[3])

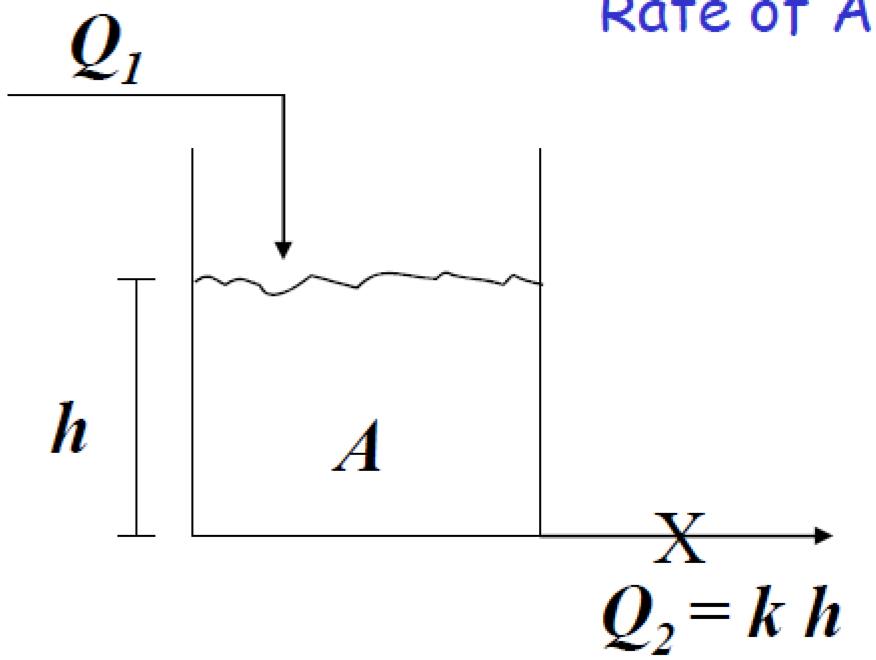
Temperature, T (°C)	Pressure, P (mmHg)
−36.7	1
−19.6	5
−11.5	10
−2.6	20
+7.6	40
15.4	60
26.1	100
42.2	200
60.6	400
80.1	760

$$P = a_0 + a_1T + a_2T^2 + a_3T^3 + \cdots + a_nT^n$$

$$\log(P) = A - \frac{B}{T + 273.15}$$

$$\log(P) = A - \frac{B}{T + C}$$

Why this course?



Rate of Accumulation = Flow Rate in - Flow Rate out

$$A\frac{dh}{dt} = Q_1 - Q_2 = Q_1 - k\,h$$

$$\Rightarrow \frac{A}{k}\frac{dh}{dt} = \frac{Q_1}{k} - h$$

$$\Rightarrow \tau\frac{dh}{dt} + h = R_1$$

Books

- Finlayson B.A., "Introduction to Chemical Engineering Computing", Second Edition, Copyright © 2012 John Wiley & Sons, Inc. https://onlinelibrary.wiley.com/doi/book/10.1002/9781118309599

- Gerald, C.F., and Wheatley, P.O., "Applied Numerical Analysis", 7th Edition, Pearson publication, 2004. http://www.cse.iitm.ac.in/~vplab/downloads/opt/Applied%20Numerical%20Analysis.pdf

Assessment and grading

- Assignments/projects/quizzes: 35%
- MTE: 25%
- ETE: 40%

Final Grade: f (your effort, involvement)

MATLAB

- https://in.mathworks.com/products/matlab.html