Process Model Formulation and Solution, 3E4

Course introduction and overview

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McMaster University

Department of Chemical Engineering

Today's class

- Course overview
- Administrative details

Acknowledgements

- **Dr. Benoît Chachuat**: formerly at McMaster, now Imperial College, London
  - All the course notes we will use were developed by him
- McMaster Advanced Control Consortium
  - Faculty: Drs. Marlin, Mhaskar and Swartz
  - Students: your TA's and other students

About myself

- Masters degree from McMaster, 2002
- Not a prof, or doctor, please
- Teach another course: 4C3, Stats for Engineers
- Also run my own engineering software company, ConnectMV
- Don't have an office on campus: email is best: dunnkg@mcmaster.ca

My objective

I hope to make this class worthwhile and practically applicable to you. Please let me know how I'm doing at any time; there will be anonymous course evaluations at least twice throughout the course for your feedback.

The general area of scientific computing

WIKIPEDIA:

"Scientific computing is the field of study concerned with constructing **mathematical models** and **quantitative analysis** techniques and using computers to analyse and solve scientific problems."

Applications of scientific computing

- Numerical simulations:
  - Reconstruct and understand known events
  - Predict future or unobserved situations

$\longleftarrow$ this is the core of 3E04!

- Model fitting and data analysis:
  - Appropriately tune models or solve equations to reflect observations

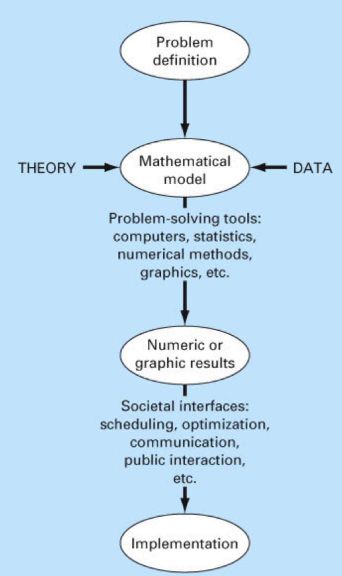
$\longleftarrow$ this is 4C03; introduced in 3E04

- Optimization:
  - Optimize known scenarios

$\longleftarrow$ this is 4G03; not treated in 3E04

Course objectives

1. **Formulate** a mathematical model in terms of algebraic or differential equations
2. Propose an appropriate **numerical method** to solve that model
3. Find a **solution** using either MATLAB™ or Python as the numerical software tool



OK, but why?

Pre-computer era

FORMULATION

Fundamental laws explained briefly

↓

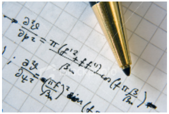
SOLUTION

Elaborate and often complicated method to make problem tractable

↓

INTERPRETATION

In-depth analysis limited by time-consuming solution



Computer Era

FORMULATION

In-depth exposition of relationship of problem to fundamental laws

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SOLUTION

Easy-to-use computer method

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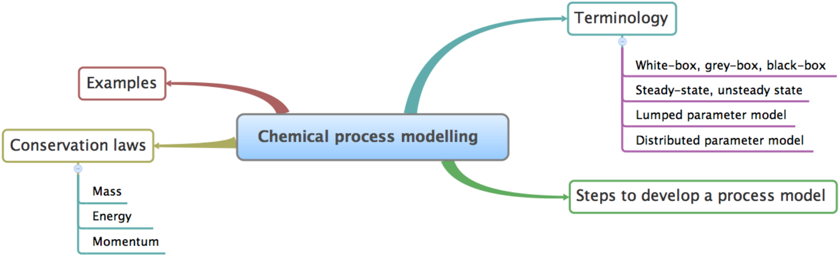
INTERPRETATION

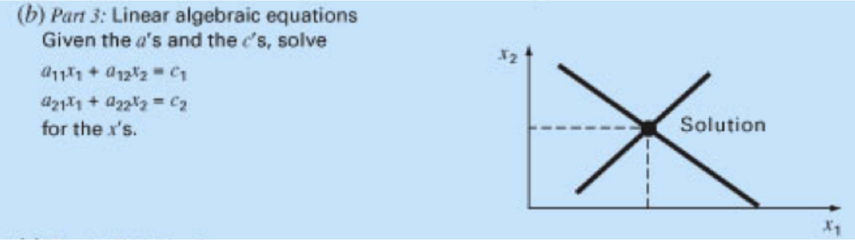
Ease of calculation allows holistic thoughts and intuition to develop; system sensitivity and behavior can be studied

Course overview: A - process modelling and computing



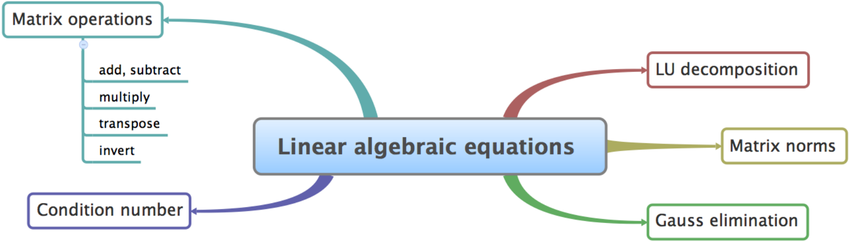
Cornerstone: The later sections will assume you can develop a model for a (chemical) process.

Course overview: B - Linear algebraic equations (LAE)



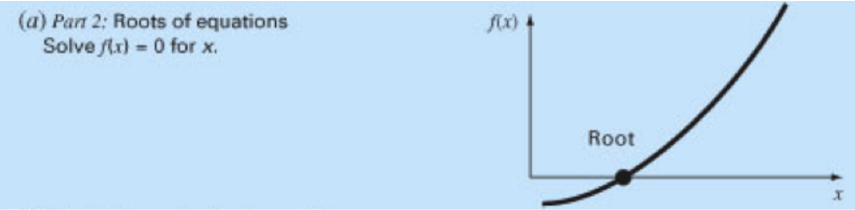
- Arise in <u>all</u> disciplines of engineering, e.g.:
  - large systems of interconnected elements
  - mass balance of a flowsheet (2D4): N equations and N unknowns

Course overview: B - Linear algebraic equations (LAE)



Cornerstone: LAE's are used in other numerical methods we will use: nonlinear systems, curve fitting, differential equations

Course overview: C - Nonlinear equation systems (NES)

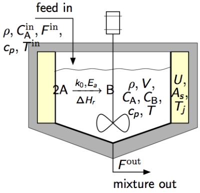


- Arises in all disciplines of engineering
  - e.g., characterize steady-state behaviour
- Allows to solve design equations for variables that are not explicit
- Both single variable equations (root finding) and multivariable equation systems

Course overview: C - Nonlinear equation systems (NES)

Consider the modeling of a jacketed CSTR, fed with a single inlet stream.

Example

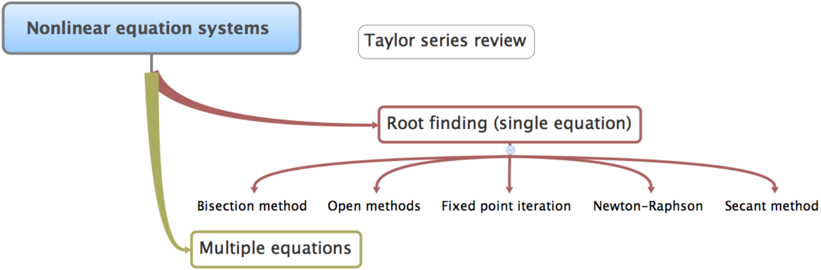


Assumptions:

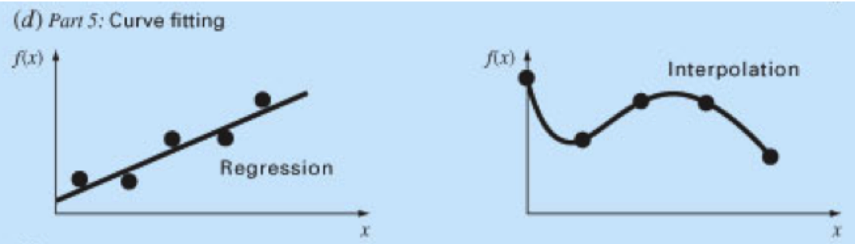
- **A1:** Perfect mixing
- **A2:** Equal inflow and outflow
- **A3:** Constant physical properties
- **A4:** Single second-order reaction
- **A5:** Neglected shaft work & non-idealities

Modeling Goals:

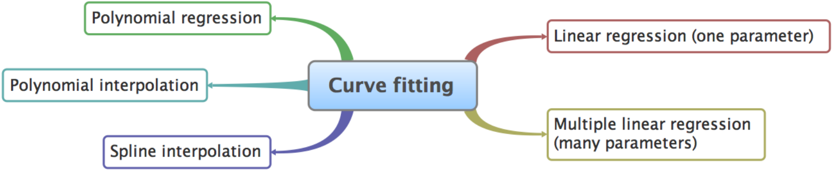
- Predict the concentration of reactant A and reactor temperature at steady-state



Course overview: D - Curve fitting



- Fit lines and curves to data points
  - Regression: measured data has error
  - Interpolation: error free data points
- Reactor design (3K4): collect data from a reaction system, regression slope is the reaction rate constant



Course overview: E - Numerical differentiation and integration

Many physical systems are modelled in terms of rates:

$$\text{Trivial example:} \qquad \text{velocity} = v(t) = \frac{d}{dt}x(t)$$

So given distance, x, at various values of t, what is $v(t)$?

Consider the modeling of an isothermal batch reactor, where an irreversible, first-order reaction A → B is taking place.

Example

$A \xrightarrow{k} B$

Experimental Data:

t [min]	c_A [mol L^{-1}]
0	1.00
5	0.84
10	0.72
20	0.57
30	0.47
45	0.37
60	0.30

Problem:

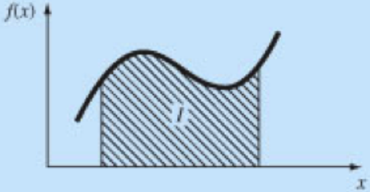
Estimate the kinetic rate k

Course overview: E - Numerical differentiation and integration

(*e*) *Part 6:* Integration

$I = \int_a^b f(x)\,dx$

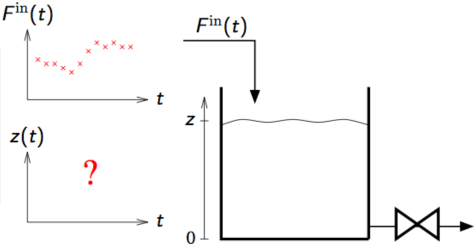
Find the area under the curve.



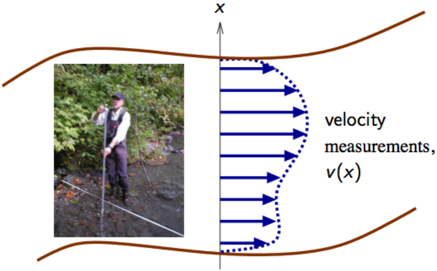
Example 1

Calculate the height of liquid after a given time:

$z(t) =$



Course overview: E - Numerical differentiation and integration



Example 2

Calculate the (constant) water flow in a river/canal:

$$F =$$

Cornerstone: a building block in numerical methods for differential equations (next section)

Course overview: F - Ordinary differential equations

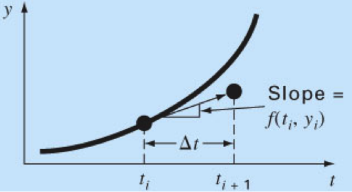
(f) *Part 7:* Ordinary differential equations

Given

$$\frac{dy}{dt} \simeq \frac{\Delta y}{\Delta t} = f(t, y)$$

solve for y as a function of t.

$$y_{i+1} = y_i + f(t_i, y_i)\,\Delta t$$

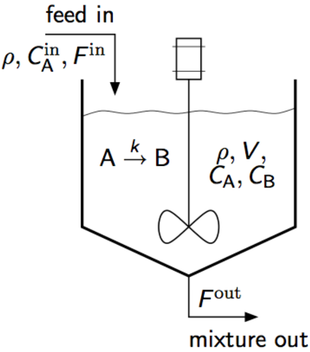


- Ubiquitous in engineering practice!
  - e.g., many physical laws written in terms of the rate of change of a quantity
- Both linear and nonlinear ODEs
- We consider initial value problems only

Course overview: F - Ordinary Differential Equations

Example

Consider the modeling of an isothermal CSTR, with a single inlet stream.



Assumptions:

- **A1:** Perfect mixing
- **A2:** Equal inflow and outflow
- **A3:** Constant liquid density
- **A4:** Single first-order reaction

Modeling Goals:

- Calculate the concentration C_A in the reactor at a given time $t \geq 0$

Administrative details

Official website:

http://modelling3e4.connectmv.com

- Announcements (also via twitter)
- Class notes: please **print out before class**
- Assignments
- Assignment solutions
- Tutorials
- Tests and exams
- Course calendar
- Grades
- Design a website logo and win a textbook

The website is your main reference for the course

Administrative: other details

Teaching assistants:

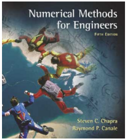
- **Elliot Cameron**, JHE 370, x22008, `cameroet@mcmaster.ca`
- **Ali Sahlodin**, JHE 370, x22008, `sahlodam@mcmaster.ca`

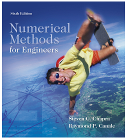
Schedule:

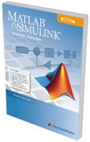
- **Classes**: Monday, Wednesday and Thursday: 17:30 to 18:20
- **Tutorial**:
  - Mon: 13:30 to 14:20: anyone (no TA available)
  - Tue: 14:30 to 15:20: last names A to K
  - Wed: 12:30 to 13:20: last names L to Z

Textbook and software:

- **Required:** Chapra & Canale, "Numerical Methods for Engineers", McGraw Hill, 5th **or** 6th Edition
- MATLAB™ Student Version: tutorial on website
- Python (free): tutorial on website







Grading

Component	Fraction	Notes
Tutorials	10%	Expect around 10 tutorial sessions
Assignments	20%	Expect 6 assignments
Take-home midterm	10%	2 to 3 days to complete the test
Written midterm	15%	A written test, lasting 2 to 3 hours
Final exam *	45%	A written exam, lasting 3 hours

* The final exam may have take-home portion as well

Grading policies

The full grading policies are on the website. Important points:

- Tutorials [**10%**]:
  - attendance not required, but ...
  - they are my office hours
  - you must hand in your solution during the time slot
  - you may give your tutorial to a friend to hand in
  - may be done by yourself, or with one other person
  - must be written or typed on paper; no email submissions
  - will be available on Monday, or earlier, on the website
  - Lastnames A to K: Tuesday, 14:30 to 15:20
  - Lastnames L to Z: Wednesday, 12:30 to 13:20

  It seems the Wednesday group has an extra day; but tutorials are meant to be started and completed within the lab session.

Grading policies

Assignments: [**20%**]

- There will be 6 assignments
- Assignment grade will be best 5 out of 6 assignments
- Can be done in groups of **at most** 4 people
- Large class: so no late hand-ins please
- 1 day late: 20% penalty; 2 days late: 40% penalty
- Stuff happens ... so 2 late-day credits per person, but not if solution already posted
- Greatest benefit: do <u>all questions</u> separately, then combine
- Defeating the purpose: each person does a question, then combine
- The purpose is to learn from each other's mistakes.
- Group work makes up 40% of the grade - use it to learn with each other.
- No sharing between groups please
- Group submissions must show all names, one hand-in per group, no separate hand-ins.

Grading policies

Tests and exams: [**70%**]

- There is a written midterm (15% of grade)
- There is a take-home midterm (10% of grade)
- Take-home test requires a computer; can be done in groups of 2 people
- The final-exam is 45% of grade
- Final might be split into a take-home portion (10%) and written (35%) portion
- Any textbook(s) and course notes are allowed in tests and exams
- Any calculator may be used during the tests and exams

Grading policies

- Please read the website for all the grading details.

Grades on the website

You can check your grades on the course website.

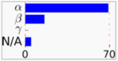
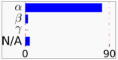
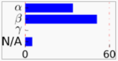
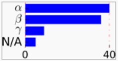
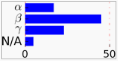
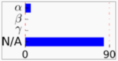
Overview

Name: R[redacted]
Student number: [redacted]
Email address:[redacted]**@mcmaster.ca**
[redacted]

Category	Weight	Your grade
Assignments	20%	[redacted]
In-class quizzes	5%	[redacted]
Mini-project	10%	[redacted]
Midterm: take-home	15%	[redacted]
Midterm: written	15%	[redacted]
Final: take-home	15%	[redacted]
Final: written	25%	[redacted]
Final grade (percentage)	**100%**	**84.4%**
Final grade (transcript record)		**A-**

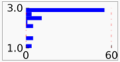
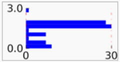
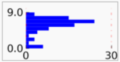
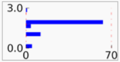
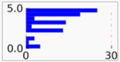
Grades on the website

Example

Category	Question	Weight [400,600]	Your grade	Class summary
Assignments		0.2	[redacted]	
Assignment 1				
	Question 1	[1.0, 1.0]	α	
	Question 2	[1.0, 1.0]	α	
	Question 3	[1.0, 1.0]	β	
	Question 4	[1.0, 1.0]	γ	
	Question 5	[1.0, 1.0]	β	
	Question 6	[0.0, 1.0]	N/A	
	Total	**[5.0, 6.0]**	**80.0%**	
Assignment 2				

Grades on the website

Another example

Midterm: written		0.15	[redacted]	
Written midterm				
	Question 1	[3.0, 3.0]	3.0	
	Question 2.1	[2.0, 2.0]	2.0	
	Question 2.2	[8.0, 8.0]	5.0	
	Question 2.3	[2.0, 2.0]	2.0	
	Question 2.4	[0.0, 4.0]	N/A	
	Question 2.5	[5.0, 5.0]	4.0	
	Question 2.6	[0.0, 2.0]	N/A