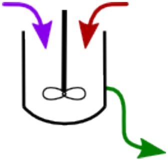
Introduction to Reactor Design

ChE 3K4



kevin.dunn@mcmaster.ca
http://learnche.mcmaster.ca/3K4

Overall revision number: 5 (January 2013)

Plan for today's class

1. Background
2. Administrative issues
3. Course contents

Background

About myself

- Undergraduate degree from University of Cape Town, 1999
- Masters degree from McMaster, 2002 (not a "doctor", please)
- Worked with a number of companies since then on data analysis and consulting projects
- Worked at GSK on a 1-year contract until June 2012
- Now working full-time at McMaster since July 2012
- Drop-in hours: Wednesday AM, Thursday PM, Friday PM
- Office is in BSB, room B105
- Arrange a meeting: `kevin.dunn@mcmaster.ca`
- Cell: (905) 921 5803 and not ~~extension 27337~~

Acknowledgments

Dr. Prashant Mhaskar

- Most of the class notes (slides) we will use are his
- Today's slides are mine; but we will use his in the next classes

Administrative issues

- TA introductions
- Announcement
- Video and audio
- Website
- References
- Software
- Expectations
- Grading

Teaching assistants

Vida Meidanshahi

- meidanv@mcmaster.ca
- JHE, room 141/A
- extension 27342
- Currently doing her Ph.D with Tom Adams

Dominik Seepersad

- seeperd@mcmaster.ca
- JHE, room 370
- extension 22008
- Currently doing his M.A.Sc with Tom Adams

Office hours: by email appointment

Video and audio

- Available for all my courses
- Purpose: for your review, and to prepare for assignments, tutorials and exams
- Might be useful if you miss a class
- As long as feasible, I will try to video record all classes
  - Try to record just myself, the board and the projector
  - Can't guarantee the quality will be very good (background noise, *etc*)
  - Video should be available within 24 to 48 hours after the class
- Audio recordings will be made available as well

Course website

http://learnche.mcmaster.ca/3K4

- Slides will be added to the site before class
- Please print slides and bring to class
- Assignments and tutorials will be posted there
- Solutions to selected/most problems will be available

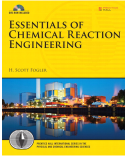
Website is the main reference for all things course-related

- expected to check it about 3 times per week (top left)
- or follow on Twitter to get updates: @3k4reactors

Reference text book

Required: Fogler, "**Essentials** of Chemical Reaction Engineering", (1st edition)

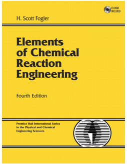
F2011



or

Required: Fogler, "**Elements** of Chemical Reaction Engineering", (4th edition)

F2006

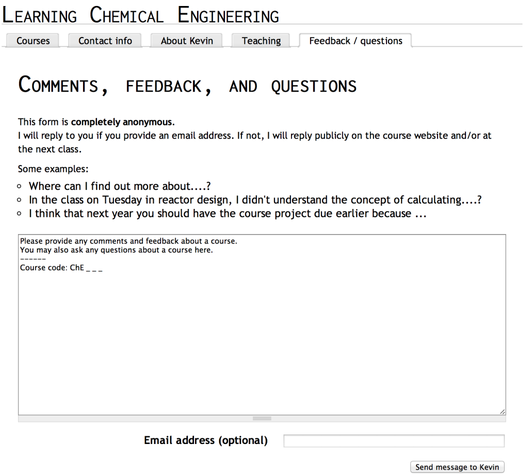


- Some other suggested books are on the course website:
  - Self-directed learning

Course feedback via Learning website

- I might not have explained something clearly;
- You didn't get a chance to ask a question, *etc*

http://learnche.mcmaster.ca/feedback-questions



LEARNING CHEMICAL ENGINEERING

Courses | Contact info | About Kevin | Teaching | Feedback / questions

COMMENTS, FEEDBACK, AND QUESTIONS

This form is **completely anonymous**.
I will reply to you if you provide an email address. If not, I will reply publicly on the course website and/or at the next class.

Some examples:

- Where can I find out more about....?
- In the class on Tuesday in reactor design, I didn't understand the concept of calculating....?
- I think that next year you should have the course project due earlier because ...

Please provide any comments and feedback about a course.
You may also ask any questions about a course here.

Course code: ChE _ _ _

Email address (optional)

Send message to Kevin

Course software

- A computer can be used for later assignments and for the course project
- I support the use of any language; Python and MATLAB in particular
- Symbolic processing: R and http://integrals.wolfram.com/
- Numerical integration: POLYMATH, MATLAB (your 3E4 scripts or `ode45`)

Let me know if you find other useful tools

Expectations outside class

- You can expect TAs and I to answer emails promptly
- If you have questions:
  1. Please email the TAs with CC to me ⟵ hopefully this solves your problem
  2. Please send from your McMaster address
  3. Set up in-person meeting with TAs or myself
  4. My office hours: Wednesday AM, Thursday PM and Friday PM

Why study reactor design?

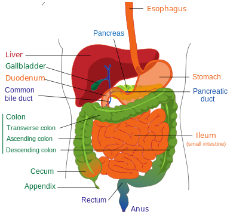
- It is an unique course to Chemical Engineering
  - Reactor Design `3K4` [reactors $\sim$ 25% of capital]
  - Separation Processes `3M,4M` [$\sim$ 75% of capital costs]

while other engineers and scientists also study:

- numerical methods
- simulation and modelling
- thermodynamics
- fluid flow and heat transfer
- statistics
- process control
- bioprocessing
- polymers
- problem solving

But this is not sufficient justification for studying a course.

There are so many "reactors" around us



- your stomach and intestinal tract
  - food ingestion
  - alcohol uptake, and breakdown
- cells: *each a complex bioreactor*
- trees: $6CO_2 + 6H_2O + \text{light energy} \longrightarrow C_6H_{12}O_6 + 6O_2$
- animals: *bioreactors*
- more than traditional reactors: (polymers and oil & gas)
  - waste water treatment
  - metals and minerals
  - food and beverage production occur in bioreactors
  - production of modern drugs

Why study reactor design?

Chemical Engineering is about "processing" material

and at the heart of any processing system is usually a reaction; converting the material to another form.

- Reactors are some of the least impressive looking units
- However, the entire plant economics and profitability are dependent on the reactor
- Get the reactor design wrong and the entire plant can be a failure/unprofitable
- Plenty of time spent on its design and optimization (years ... not months are often taken)

Why study reactor design?

The outcome of a “reactor design”: multi-compartment autoclave

4.7m inside diameter, 25m long

[Hydrometallurgy of Nickel and Cobalt 2009, The Metallurgical Society of the Canadian Institute of Mining, Metallurgy and Petroleum, Symposium]

Why study reactor design?

But most usefully, and the most likely case you will find:

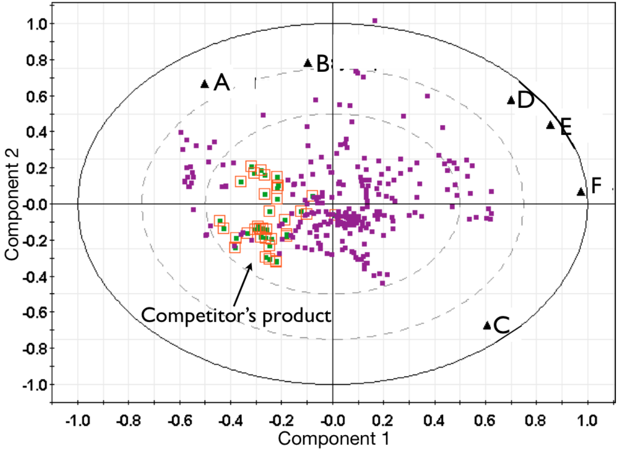
You are working at an existing plant, with the reactor running for many years and producing product profitably.

1. A recession hits (e.g. 2007/2008/2009), and you need to scale back. Less demand for your product.
   - What reduced flow rate do you operate at?
   - Will the reaction still go the required conversion?

2. There is increased demand for your product, right away. No time to design, install and commission a second reactor.
   - What increased flow rate do we operate at?
   - What will happen to side-reactions and impurities?
   - Can we still get the same conversion in the fixed-size reactor?
   - Maybe change the catalyst, or operate at a higher temperature?

Why study reactor design?

3. Competitors from another country/company/using a different technology are making the same product, at a cheaper price.
    - Can you operate at lower temperatures to save money?
    - What can you adjust to increase conversion?
    - How can you further reduce impurities in the outlet, creating a more valuable, consistent product for your customer?



What is “Reactor Design”?

How to produce a specified product, at a given rate, from known reactants.

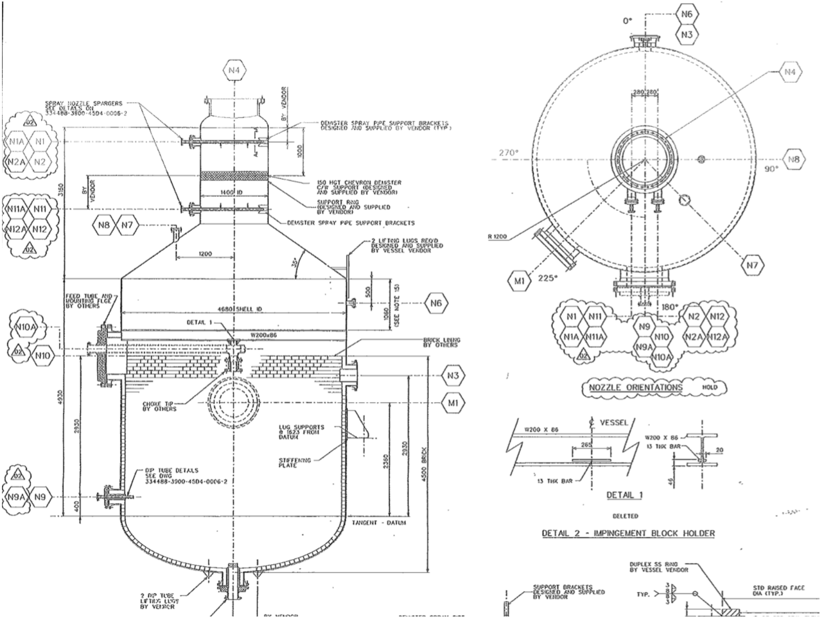
Decisions we have to make

- What type of reactor do we use? Batch, plug-flow, tank, packed-bed, others...
- Will we operate isothermally, adiabatically, or a hybrid?
- At what temperature, pressure, compositions and flows do we operate?
- Which phases are present: liquid, solid, gas, or a hybrid?

What we need to know

- The size of the reactor
- Composition of products leaving
- Temperatures in the reactor
- Pressure in the reactors, and pressure drop across it

What we won't be studying: "Design of reactors"



[*Thanks Dad!*]

What we won't be studying: "Impellers and internals"

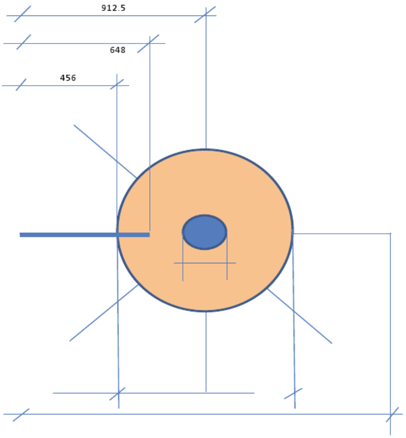
NEW IMPELLER - DESIGN CALCULATIONS

	Standard	Selection
Number of blades =	6	8
D/T (Impeller Diameter/Vessel diameter) =	0.33	0.365
h/D (Blade Height/Impeller Diameter)	0.20	0.320
w/D (Blade Width/Impeller Diameter) =	0.25	0.355
Np	5.75	
C/D	3.00	1.00
Effect of number of blades:		
Np/Np_{std} = (No of blades/6)^0.7	1.00	1.22
Effect of Blade Height:		
Np/Np_{std} = ((h/D)/(h/D)$_{std}$)^1.45	1.00	1.98
Effect of Blade Length:		
Np/Np_{std} = ((w/D)/(w/D)$_{std}$)^0.33	1.00	1.12
Np/Np_{std} for Proximity Factor C/D	1.10	0.90
Np/Np_{std} for Underbaffling Swirl Factor	1.00	0.85
Np Power Factor	6.33	11.95

Motor Power,kW	400
Fraction Motor at Full load, %	0.96
Gearbox efficiency	0.98
k-factor (gassed power/ungassed power)	0.64
Impeller Speed, rpm	68.5
Impeller Speed, rps	1.14
Vessel Diameter, mm	5000
Impeller Diameter, m	1825
Disc Diameter, mm	913
Blade Height, mm	584
Blade Width, mm	648
Height from floor to Ruston Impeller	1825
Pulp SG, kg/L	1.42

IMPELLER DIMENSIONS

NOT TO SCALE

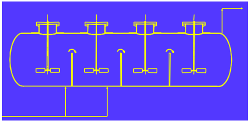


[*Thanks Dad!*]

What we won't be studying: "Materials of construction"

[*Thanks Dad!*]

What we won't be studying: "Internals"



[*Thanks Dad!*]

What we won't be studying: "Externals"

[*Thanks Dad!*]

What we won't be studying

- Design of the internals: heating/cooling tubing, flanges, baffles, motors, flanges, clean-in-place systems
- Design of systems with catalysis and mass-transfer limitations

What we won't be studying

- Non-ideal behaviour that is present in most systems
  - though we will introduce it near the end of the course
  - Does this CSTR obey all the assumptions?

How this course is structured

There are 8 main sections, spread over 12 weeks

1. Mole balances
2. Conversion and reactor sizing
3. Rate laws and stoichiometry
4. Isothermal reactor design
5. Collection and analysis of rate data
6. Multiple reactions
7. Steady-state nonisothermal reactor design
8. Distributions of residence times

Grading

What we look for in the grading is demonstration that you/group:

1. understand the concept,
2. have the ability to apply the concept to new instances,
3. think creatively about problems,
4. my questions are seldom "plug-and-chug",
5. numerical accuracy,
6. grammar and spelling.

Grading for assignments

- *Appropriate* group work is highly encouraged
  - Up to 30% of course grade
  - *Learn with each other*
  - Assignments and project done in groups of 2, or by yourself
  - Hand these in assignments as one submission
- Late grading
  - -30% per day
  - 2 "late day" credits for assignments
  - solutions posted after $\approx$ 2 days of due date
- Assignment grading:
  - No make-ups for assignments
  - Counts **15%** of course grade
  - All assignments will be used for the grade
- Assignment dates: see website
- http://learnche.mcmaster.ca/calendar

Group-based assignments

- "Appropriate" group work is highly encouraged (about 30% of course)
- Learn with each other: groups of 2, no larger

- Optimal group work: *an example of one approach*
  - Sarah and Brad work on an assignment
  - Both Sarah and Brad do **all questions** in draft: quick notes at home, on the bus, *etc*, ± 4 days before assignment due
  - Meet in the library next day and go over each other's notes
  - Explain to the other why you disagree
  - e.g. Sarah sees a mistaken interpretation in Brad's work
    - She explains why it is a mistake to Brad: Sarah learns
    - Brad also learns: he's heard this in class, and from Sarah now
    - If neither can resolve it? speak with TAs or Kevin
  - Write up a joint solution; e.g. Sarah Q1 and 2, Brad does Q3
  - Both review it before submitting

- Other approaches are possible: your group decides
- What doesn't work: Sarah does Q1 and Q2, Brad does Q3; staple and submit; no group review
- **Do not share files or written work** *between* groups

Grading for exams and project

- Written midterm on 13 February: **20%**
  - it is optional
  - there is no make-up
  - if you miss it, your final counts more
  - covers all material up to 12 February
- Written final exam: **50%**
  - Covers all material
- Midterm and final exam:
  - Open notes – anything on paper is allowed
  - No electronic devices unfortunately
  - Any calculator
- Project due on 27 March: **15%**
  - Requires computer software
  - Can collaborate, **but only within your group**: not between groups

Electronic submissions

You may submit assignments electronically

- via Google Docs only
- Share your document with special gmail addresses:
  - `kgdunn@gmail.com`
  - `mac.che.3k4@gmail.com`
- More details on the course website
- TAs will grade it electronically
- Saves paper, allows group collaboration

Important dates

- 13 February mid-term
- 27 March: project due
- 08 April: last (review) class
- April: final-exam

- Something due every 2nd week: see calendar