CHEE 641 Chemical Reaction Engineering
Winter 2021

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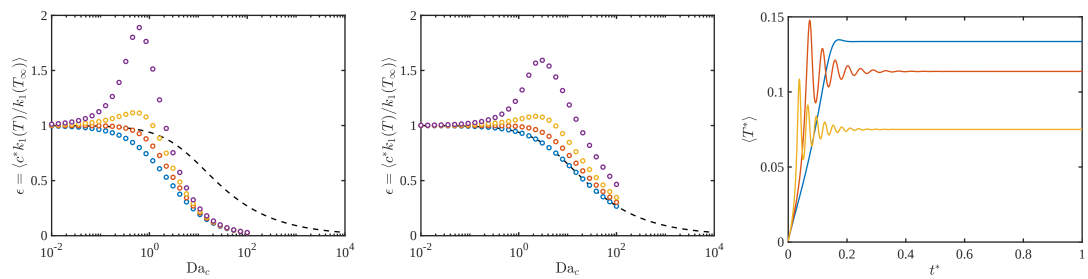
June 11, 2021

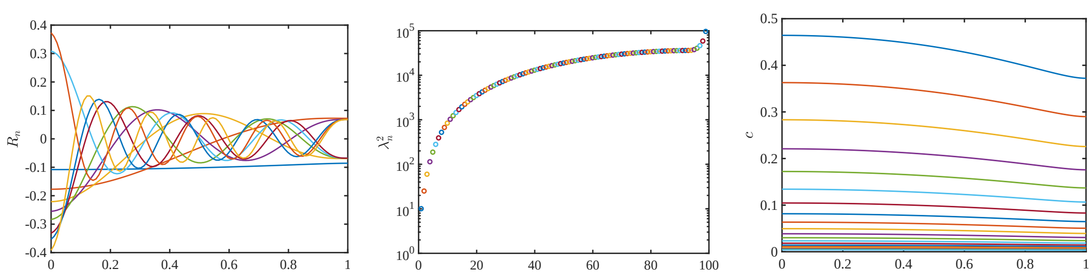
CHEE 641 course-evaluation metrics (2021):

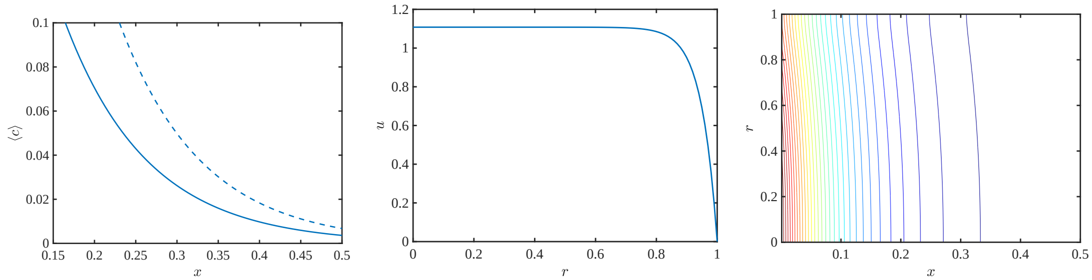
- Q1. Overall, this is an excellent course. Hill 4.3 (DCM 3.6)
- Q2. Overall, I learned a great deal from this course. Hill 3.8 (DCM 3.8)
- Q3. Overall, this instructor is an excellent teacher. Hill 4.5 (DCM 4.1)
- Q4. Overall, I learned a great deal from this instructor. Hill 4.3 (DCM 4.1)

DCM = department course mean.



Exploring external and internal mass-transfer limitations on non-isothermal catalysis (Bi ~ 1, $\gg 1$).





PFRs with radial dispersion. (a) Eigen-functions. (b) Eigen-value spectrum. (c) Radial concentration profiles. (d) Average concentration with (solid) and without (dashed) radial dispersion. (e) Axial velocity profile (Brinkman medium).

The following topics were covered in 2021:

1. *Introduction/undergraduate reaction engineering review.* Mole conservation; reaction rate; elementary and non-elementary reactions; gas- and liquid-phase concentrations; Arrhenius rate law; reversible reactions; competing reactions.

2. *Pressure effects.* Ergun, Darcy-Weisbach, Colebrook-White equations and their application to PFRs; pressure/density and temperature effects on fluid properties and diffusivities; pressure drop (density and volumetric flow) in an isothermal packed bed; Darcy and Brinkman velocity profiles in pipe flows.

3. *Isothermal reactors.* Modelling plug flow (PRF), continuously-stirred/mixed-flow tank/ (CSTR/MFR), batch, semi-batch, and fluidized-bed (FBR) reactors; conversion, specificity and yield; Levenspiel plots; degrees of freedom analysis; conversion average residence time in reactors with volume change; recycle reactors, non-linear Denbigh reactions.

4. *Non-ideal reactors.* Residence time distribution; dispersion, tanks-in-series; micro- and macro-fluids; states of aggregation and segregation; early and late mixing; maximum mixedness model.

5. *Equilibrium reaction thermodynamics.* Equilibrium constant and its temperature dependence; derivation of the van't Hoff equation; temperature and pressure effects on reversible reactions; connection between the equilibrium constant and kinetic rates.

6. *Competing reactions in isothermal reactors.* Strategies to optimize reactors based on kinetic, thermodynamic and mixing considerations; measures of yield.

7. *Reaction mechanisms and catalysis.* Non-elementary rate laws; intermediates; quasi-steady-state approximations; mechanisms of Langmuir-Hinshelwood and Eley-Rideal.

8. *Particulate catalysis and reaction kinetics.* Reaction-diffusion model; extending the text-book Thiele modulus model to address additional heat- and mass-transfer limitations, temporal, and non-isothermal effects.

9. *Non-isothermal reactors.* Detailed derivation of the dynamic energy balance for reacting and heat-transfer fluids, and its application to a variety of control volume/reactor types.

10. *Non-isothermal PFR.* Case study and model.

11. *Non-isothermal CSTR.* Case study and model.

12. *Non-isothermal, non-isobaric PFR.* Case study and model.

13. *Dynamics and stability.* Multiple steady states; linear stability; stabilizing open-loop unstable operation with PID control.

14. *Membrane reactors.* Conversion, selectivity and yield. Steady-state PFR: Gas-phase $A+B \rightleftharpoons C$ (w/ C-permeable membrane, and co-/counter-current heat-transfer fluid). Steady-state PFR: Gas-phase $A + B \to D$, $D + B \to U$ w/ D-permeable membrane, and co-/counter-current heat-transfer fluid).

15. *Laminar-flow parallel-plate reactors.* Laminar-flow parallel-plate reactor with 1st-order reaction at bottom surface. Analysis based on a reactive Graetz model (eigen-value/eigen-function decomposition) and dimensionless parameters. Differential-reactor limit, and integral-reactor analysis.

16. *Bioreactors.* Enzymatic reactions and mechanisms (Michaelis-Menten), dynamic models for cells (empirical Monod and variations), coupling to substrate and product balances (incorporating cell growth, death, maintenance and inhibition). Fermentation chemostat and dynamic tank reactors. Interpreting VO2 max dynamics using a dynamic physiological model (linearized state-space analysis, two time-constants).