**Analysis and modeling of the great *ideas* of chemical engineering CBE 34xxx**

Proposed as a *Chemical Engineering Elective,* 3 credits.

Prereqs: CBE 20258, 20260, Math 20580, Chem 20273. (or permission of Instructor)

Summer, 2020. To be taught remotely during (+ pre-week?)June 1- July 24. T/R 7-8:30PM (time subject to some student polling).

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One can find many lists of the *greatest chemical engineering achievements*. We might include U235 isotope separation, ultra-pure silicon, catalytic cracking, …. or the amazing efficiency and safety of ammonia plants[1]!..

For this course, the underlying theme will be topics and ideas that that continue to be central to chemical engineering. For example, chemical engineers are the dominant intellectual drivers of phase and chemical equilibria, analysis on "small" scales of mass and heat transfer and fluid flow — particularly where external field forces are present. Chemical kinetics and catalytic reactions, molecular and nanostructural understanding of solid materials are some other topics where chemical engineers are the dominant intellectuals.

Besides these and other specific technology examples, chemical engineering also (almost uniquely) employs some intellectual powerful tools such as, *dimensional analysis*, *concept of a steady-state* (as distinct from "equilibrium" ), *control volumes*, optimization in terms of *operating and capital costs,* multiple stages to accomplish reactions and separations[2], and a favorite of the instructor, what can be learned by taking any system or thought to its limits.

This course will balance explanation of these topics[3], with using them as examples of analytical and numerical solutions of (1) multiple algebraic equations, (2) single or multiple odes and (3) single or multiple pdes. By using *Mathematica* and the "library" of 25 years of examples on these and many other topics, it will be possible for students to

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[1] The number of sessions titled "*Safety in Ammonia Plants"* at the *Annual AIChE* meeting, has dropped over the years, but back when there were only a couple hundred total sessions, there were 5 or 6 such sessions. The 1989 Annual meeting was in San Francisco only a few weeks after the *Loma Prieta* earthquake. Aftershocks were still occurring which led to one of the all time best *Roger Schmitz* lines… "if it starts shaking real hard, I am heading for an Ammonia Plant — it must be the safest place on earth!"

[2] It is not hard to find papers in *Science* or *Nature* gushing over a specific value of a partition coefficient — when knowing that such processes could be done with multiple countercurrent stages — other factors are actually more important.

[3] which will be explained in depth that matches their nominal slots in the undergraduate curriculum.

explore each of the topics both qualitatively and quantitatively using numerical and analytical solutions — without the need to code and debug all of the algorithms or to learn how to solve a PDE with LaPlace Transforms or Eigenfunction analysis.

No doubt that in additional to these classic topics, we will feel compelled to examine some health - related topics such epidemic modeling, linear and nonlinear time series techniques to examine “heart rate variability”, energetic analysis of bacteria with applications to antibiotic resistance and transport in biofilms.

The format will be on-line synchronous lectures, with 1/2 of the grade from individual weekly homework, 1/2 from an individual/small group project.

**(Tentative) Topics:**

June 2, 4: *Dimensional Analysis* (Linear algebra, emergence of parameters and perturbation solutions)

Jun 9, 11, 16: *Differential Equations of Transport Phenomena* (examination of the underlying phenomena, scaling/ simplification of equations and emergence of parameters, analytic solutions, numerical solutions)

Jun 18: *Phase Equilibria*. ( Solving cubic equations of state and activity coefficient models)

June 23, 25: *Chemical Reaction Kinetics and Mechanisms* (Fitting rate expressions to chemical and biological data, Arrhenius kinetics, solving equations mass and energy equations for batch, stirred tank and plug flow reactors)

June 30, July 2: *Separation Processes* (staged and continuous contact operations, systems of linear equations, use of differential control volume)

July 7: *Optimization* (Objective functions — cost trade-offs, Linear Programming)

July 9: *Stability of Flows and Processes* (Linearization of ODEs and PDE using Fourier modes and solution of eigenvalue problems.)

July 15, 17: *Time Series Analysis* (Fourier spectral and nonlinear techniques for process, environmental and physiological data)

July 21: *Molecular dynamics simulation* (Calculation of continuum properties)
July 23: Additional topics from medicine and physiology

Some possible additional/substitute topics:

Data mining, predictions of general “law”s… and its limitations

Modeling various cooking processes.