Course Syllabus

CHE656: Process Analysis and Modeling

Semester II, 2023
URL: https://www.cheps-kmutt.com/che656

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Course Description:

This course is a complement to CHE654: Computer Application for Chemical Engineering Practice. The course emphasizes two additional vital skill areas that chemical engineers need, especially those in process engineering, namely modeling and optimization. Modeling allows a chemical engineer to study a physical or chemical system/process and derive a mathematical model in the forms of algebraic equations and/or differential equations that best describe the performance of the system. This mathematical model can then be solved by hand or by solvers in MATLAB. In addition, fundamental concepts of optimization are introduced in this course which is an important element in process simulation. Optimization allows chemical engineers to maximize or minimize a certain cost-based or performance-based objective function, such as maximizing the total profit or minimizing energy consumption in a process. Basic principles of optimization will be first introduced, which include optimization of single variable, multiple variables, unconstrained optimization, constrained optimization, linear programming, nonlinear programming, etc. Real applications involving chemical systems will be used as illustrations of the different optimization techniques.

This course once again consists of 2 parts: lecture and design projects (to enhance student soft skills). In design projects, students will work in teams and make regular presentation with the same format as that in CHE654. Each design project consists of two problems which will involve solving an open-ended AIChE Student Design Competition Problem and studying a given optimization metaheuristics and coding them in MATLAB to solve a variety of optimization problems including those encountered in chemical engineering.

This course is essential to understanding CHE659 (Optimization of Chemical Processes) in which process optimization using A+ will be emphasized.

You will be graded based on the following areas:

Homework (8 sets) & Tutorials (2 sets)	15%
Midterm (4 hours)	30%
Final Exam (4 hours)	30%
Design Project (team)	25%

- Presentations (10%)
- Final Report (15%)

Note that homework assignments and solutions are to be downloaded from my website at www.cheps-kmutt.com or from KMUTT LEB2. Their due dates will be posted there as well.

Finally, this course is an OBEM (Outcome-based Module) course, which means it is structured based on a number of learning modules. A set of assessment tools and criteria will be used to judge if a student passes each learning module. Details about OBEM will be discussed during the first lecture of this course.

Textbooks and References:

1. *Modeling and Simulation in Chemical Engineering,* by Roger G.E. Franks, John Wiley & Sons, Inc., New York, 1972.
2. *Computational Methods for Process Simulation,* 2nd Edition, by W.F. Ramirez, Butterworths, Boston, 1997.
3. *Applied Numerical Methods for Engineers Using MATLAB and C*, by Robert J. Schilling and Sandra L. Harris, Brooks/Cole, 2000.
4. *Applied Mathematics in Chemical Engineering*, by H.S. Mickley, T.S. Sherwood, and C.E. Reed.
5. *Applied Mathematical Programming*, by S.P. Bradley, A.C. Hax, and T.L. Magnanti, Addison Wesley, 1977.
6. *LINDO User's Manual*, by LINDO Systems Inc., 1999.
7. Supplementary Lecture Notes at www.cheps-kmutt.com.
8. *CHE656 Exercise Problems* by Dr. Hong-ming Ku, 2023.

The following is an outline of topics to be covered in this course:

Part 1:

1) Basic Modeling
   - Hydraulic tank
   - Enclosed tank
   - Mixing vessel
   - Mixing with reaction
   - Simultaneous mass and energy balances
   - Continuous-flow boiling system

2) Multicomponent Vapor-Liquid Equilibrium
   - Vapor-liquid equilibrium
   - Boiling operations
   - Batch distillation

3) Reaction Kinetics

Part 2:

4) Basic Concepts of Optimization

5) Optimization of Unconstrained Single Variable

- Indirect methods vs. direct methods
  a) Region-elimination methods
  b) Newton-Raphson and Quasi-Newton methods
  c) Secant method
- Using *fminbnd* in MATLAB

6) Unconstrained Multivariable Optimization
   - Indirect methods vs. direct methods
     a) Steepest descent
     b) Sequential simplex
     c) Conjugate search and conjugate gradient method
   - Using *fminunc* and *fminsearch* in MATLAB

7) Linear Programming
   - Simplex algorithm
   - Using LINDO

8) Nonlinear Programming with Constraints
   - Using *fmincon* in MATLAB

9) Discrete and Staged Optimization
   - Integer programming
   - Using LINDO

<u>Part 3</u>:

10) Design Projects