Course Syllabus

CHE654
Computer Applications for Chemical Engineering Practice
Semester I

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Web Page: https://www.cheps-kmutt.com/che654-year1-semester1

Lecture Hours: To be announced

Course Description:

Computers have become an indispensable tool in the profession of chemical engineering. Computers are often used to perform complex and iterative calculations typically encountered in heat and mass balancing, sizing and costing calculations, sensitivity analyses, and optimization of a chemical process.

The objective of this course is to give a broad coverage of the field of computer applications to chemical engineering, with emphasis on steady-state process simulation and using MATLAB as an engineering computational tool. Both theoretical foundations and practical applications in flowsheeting will be presented and discussed. For practical applications, students will learn how to use a steady-state process simulator called ASPEN Plus (A+) to model and solve real-life processes and MATLAB to solve complex chemical engineering problems.

The course uses a combination format of lectures, hands-on workshops, and some computer assignments. Points will be kept for homework, a midterm, and a final exam with the following distribution:

The course is divided into 3 parts – process simulation with A+, solving equations with MATLAB, and design projects. The distribution of points will be:

A+ and MATLAB (75%)
- 9 homework assignments and 7 tutorials (15%)
- Midterm (30%)
- Final Exam (30%)

Design Projects (25%)
- Presentation (10%)
- Final Report (15%)

References:

1. *Integrated Design and Simulation of Chemical Processes* 1st Edition by A.C. Dimian, Elsevier Science, May 2003.
2. *Uncovering the Realities of Simulation Part I* by Rajeev Agarwal *et al.* Chemical Engineering Progress, May 2001, pp. 42-52.
3. *Uncovering the Realities of Simulation Part II* by Rajeev Agarwal *et al.* Chemical Engineering Progress, June 2001, pp. 64-72.
4. *Don't Gamble with Your Physical Properties* by Eric C. Carlson, Chemical Engineering Progress, October 1996, pp. 35-46.
5. *Don't Let Recycle Stream Stymie Your Simulations* by Ryan C. Schad, Chemical Engineering Progress, December 1994, pp. 68-76.
6. *ASPEN Plus V7.3: Getting Started Building and Running a Process Model* (pdf file) by Aspen Technology, Inc.
7. *Modeling and Simulation in Chemical Engineering,* by Roger G.E. Franks, John Wiley & Sons, Inc. New York, 1972.
8. *Computational Methods for Process Simulation*, 2nd Edition, by W.F. Ramirez, Butterworths, Boston, 1997.
9. *Applied Numerical Methods for Engineers Using MATLAB and C*, by Robert J. Schilling and Sandra L. Harris, Brooks/Cole, 2000.
10. *Applied Mathematics in Chemical Engineering*, by H.S. Mickley, T.S. Sherwood, and C.E. Reed.
11. *Introduction to MATLAB*, by Prof. Gregory J. McRae, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139.
12. *MATLAB Programming Style Guidelines*, by Richard Johnson.
13. https://www.cheps-kmutt.com/che654-year-1-summer to download more references and homework assignments.

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

1. Simulation of Continuous Processes
   - History and fundamentals of process simulation
   - Partitioning and tearing a flowsheet
   - Tutorial #1

2. Processing Simulation with ASPEN Plus
   - Introduction to the ASPEN Plus Simulation Package
     - ❖ Features of ASPEN Plus
     - ❖ Introduction to the ASPEN Plus Graphical User Interface
     - ❖ Survey of unit operation models
     - ❖ Tutorial #2
   - Multistage Separation
     - ❖ RADFRAC: Rigorous rating and design fractionation model
     - ❖ Examples of rigorous column models
   - Flowsheet Calculations and Model Analysis Tools
     - ❖ Sensitivity analyses
     - ❖ Design specifications and calculator blocks
     - ❖ Tutorial #3
   - Physical Properties

- Overview of physical property system
- Property model specifications
- Property data requirements and input
- Special topics
- Physical property analysis
- Tutorial #4

- Flowsheet Convergence
  - Tutorial #5

3. Numerical Solutions Using MATLAB
   - Overview and simple arithmetic capabilities
   - Matrix manipulations
   - Nonlinear Algebraic equations
   - Ordinary differential equations
   - Programming in MATLAB

4. Plant Design Projects
   - See the Design Project Statement