Course Syllabus

CHE494 Special Topics III
Chemical Process Simulation and Applications
Semester 1, 2023

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Lecture Hours: Friday, 1:30 – 4:30 pm

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. Both theoretical foundations and practical applications in process simulation and flowsheeting will be presented and discussed. For practical applications, students will learn how to use a steady-state process simulator called ASPEN Plus to model and solve real-life processes.

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:

Homework Assignments	20%
Midterm Exam	40%
Final Exam	40%

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.

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

1. Introduction to Process Simulation
   ❖ Applications of process simulation
   ❖ History of process simulation
   ❖ Different approaches to process simulation

2. Modules and components in a process simulation package

3. Tear streams and recycle streams in process flowsheeting

4. Introduction and Features of the ASPEN Plus Simulation Package

5. ASPEN Plus Graphical User Interface and running a simulation model

6. Elementary modules and mass balance only in ASPEN Plus
   ❖ Mass balance with standard input
   ❖ Mass balance with design targets (design specifications)

7. Survey and examples of important unit operation models

8. RADFRAC: Rigorous rating and design fractionation model

9. Flowsheet Calculations and Model Analysis Tools
   ❖ Sensitivity analyses
   ❖ Calculator blocks

10. Physical Properties in ASPEN Plus
    ❖ Overview of physical property system
    ❖ Choosing a proper method
    ❖ Multiple property methods in the same flowsheet
    ❖ Property parameters and input
    ❖ Tabpoly data
    ❖ Property constant estimation system (PCES)
    ❖ Property analysis
    ❖ Property sets (Prop-sets)

11. Flowsheet Convergence