

416f Incorporating Chemcad with Process Design: a Laboratory Method

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Chemical engineering students who enter industry jobs are finding that companies are commonly using simulation packages. For students at Mississippi State, the use of simulation packages was left up to the teachers of the individual classes. With no standardization, some students graduated Mississippi State with minimal simulation experience. With the realization that a hole existed in the students' education, a new class was formed as a way to introduce simulation to every student. A senior design class, Process Design, is used to teach costing, troubleshooting, and basic principles needed to design chemical processes and plants. With the addition of a one hour laboratory, the simulation package, ChemCAD, could also be taught.

ChemCAD is a common simulation package available to universities and industry. The program is loaded with features, which means that a multiple week course is needed. The lectures were divided into different topics, to cover as much of the core chemical engineering curriculum as possible. To ensure all of the students began at the same place, the course began with a lecture on using ChemCAD, which included adding components, drawing a flowsheet, and running the simulation. The Thermodynamics package within ChemCAD is very involved, so a two week set of lectures was used to convey the importance of thermodynamics. Heat exchangers, distillation columns, multiple types of reactors, controllers, and component separators were also taught, with one topic covered per laboratory session. Two of the biggest features of ChemCAD are the sensitivity analysis and optimization. Sensitivity analysis, or the ability to determine how a process reacts to a change in operating parameters and design variables, was covered by one laboratory session. Optimization, that helps determine the best values for a given variable, was covered after the lecture on sensitivity analysis, since sensitivity analysis is necessary to determine what variables and parameters affect the process. Finally, other features of ChemCAD were covered, which included exporting data to Excel, creating and running recycle loops, understanding and modifying convergence parameters, and producing spec sheets and environmental reports.

For the students to learn how to use ChemCAD and the nuances of the program, homework was assigned each week. As an example, the thermodynamics package consisted of two unique homework sets. The first week used several different mixtures, such as isopentane and *n*-pentane, propane and benzene, and MIBK and water. These mixtures were graphed using multiple different models, to demonstrate that what works for one compound will not work for another compound. The second week consisted of a problem that resulted in ChemCAD's thermodynamics wizard choosing an incorrect thermodynamic model. The students then had to identify which model would be most accurate for the system being designed. Homework was also assigned for the other lectures, with some of the homework used to help the students understand sensitivity analysis and optimization. At multiple times during the semester, projects were given that were designed to incorporate material from the Process Design class and the laboratory.

Since ChemCAD has many features and unit operations that could not be covered, the laboratory's purpose was to teach the students to use ChemCAD and troubleshoot homework and design projects. The expectation is that the students will be prepared to use ChemCAD in their industry jobs.