A Just-in-Time Pedagogical Approach for Numerical Methods in Chemical Engineering

During 2009 the Department of Chemical Engineering at the University of Texas at Austin made a major revision in the pedagogy for ChE 348, the required sophomore level numerical methods course in chemical engineering. This change was undertaken because both faculty and students expressed dissatisfaction with the current traditional numerical methods course because it does not reflect the way numerical methods software is used by practicing chemical engineers today. The ChE 348 committee decided to change the format of the course to a just-in-time (JIT) learning approach applied to a series of case studies, each of which presents an engineering design problem to be solved. In JIT the instructor presents a multi-faceted engineering problem to be solved. Then she/he leads the class to identify what numerical methods are needed to solve the problem and then covers the background so students can attack the problem. This is different from the "theory first, then graph?" pedagogical approach. The design problems span the undergraduate curriculum covered in the junior and senior years, namely fluid flow, heat transfer, mass transfer, reactor design, thermodynamics, and separations. Table 1 shows how the important concepts in numerical methods map to applications (motivational case studies). The faculty committee does not believe there is a textbook available that fits the needs of the restructured course, hence we have developed instructional materials in a modular format to use in the course to supplement the extensive set of presentation slides developed by the faculty who have recently taught the course. Over time other modules will be added so that there will be a library of possible case studies that a professor can select. The case study problems will include examples from major areas of chemical engineering, such as chemical processing/refining energy, materials processing/design, biomedical engineering, bioengineering and environmental / sustainability.

We believe that both faculty and students now have a higher level of satisfaction with the new course, which was taught first by Professor Bonnecaze in Spring, 2010. Other chemical engineering courses will benefit from having a more effective numerical methods course where instructors in those courses will be able to add numerical exercises to those courses to reinforce the concepts. The pedagogy developed in this course (case study approach) could be transportable to other ChE departments who teach an undergraduate numerical methods course.

Table 1
Case Study Approach to ChE 348 (Numerical Methods)

Numerical Method/Modeling Technique for Students to Learn	Case Study Problem to Motivate Learning Methods
Solution of Linear Algebraic Equations	Case Study I: Multicomponent Material Balance for Separation Process with Recycle
Solution of Non-Linear Algebraic Equation	Case Study II: Phase Equilibrium
Solution of System of Non-Linear Algebraic Equations	Case Study III: Reactor Train of CSTRs
Solution of Ordinary Differential Equations – Initial Value Problem	Case Study IV: Runaway Reactor Operational Sensitivity
Solution of Partial Differential Equations	Case Study V: Oxygen Scavenging Membrane for OLED Packaging
Solution of Ordinary Differential Equations – Boundary Value Problem	Case Study VI: Non-linear Reaction in a Catalyst Pellet
Optimization	Case Study VII: Parameter Estimation of Kinetic Data

The case study IV on runaway chemical reactors focused on the accident that occurred at the T2 Laboratories in Jacksonville, Florida on December 19, 2007. The class presentation for this case study is attached here. This accident was analyzed by the U.S. Chemical Safety and Hazard Investigation Board (CSB), which provided excellent resources for this case study. Among the recommendations of the report was the incorporation of reactivity hazard awareness into the curriculum of B.S. chemical engineers. The addition of this case study is a first step along this path. The students also completed a team design project based on computational simulation. In the first version of this case study driven course, the student teams were charged with a) creating a simulation tool for the design of polymeric oxygen scavenging barriers for packaging organic electronic material and b) using the tool to specify the design of such a barrier material to meet specific functionalities.

Problem Set 7