World wide Web-Based Modules for Introduction of Molecular Simulation into the Chemical Engineering Curriculum (NSF Grant 9752243)

Richard Rowley, Brigham Young University

This grant involves seven co-PIs from academic institutions around the country, all experts in molecular simulations, and was funded in 1998 as a three year grant managed by the CACHE Corporation. The objective of the grant is to develop WWW-based modules to facilitate introduction of molecular simulation into the chemical engineering undergraduate curriculum. These teaching modules are to be integrated directly into chemical engineering core undergraduate courses, supplying for the instructor and the student the appropriate linkage material between macroscopic concepts currently taught in these courses and molecular simulations designed to aid student understanding of the molecular underpinnings of the phenomena. Modules are centered around Java Applets that run the molecular simulations and provide an "experimental" simulation platform for students to explore concepts. In addition, modules contain instructor materials, fundamental tutorials, student problems, and assessment materials.

During the second year of the grant, we found that development of web applets in Java was a problem for faculty members with expertise in molecular simulations. This became a serious problem as we tried to expand the development of these modules to additional developers at other universities. People interested in working with us to develop simulation modules simply did not have the JAVA skills necessary to produce a quality product. Additionally, the modules produced lacked cohesion and versatility necessary for adoption by faculty and use by students to explore concepts in an "experimental" mode. To remedy this, we stopped work on individual modules and concentrated on programming a module-development environment called Etomica. Etomica is a fully functional, browser-based module development environment in which modules can be put together using click, drag-and-drop, and selection capabilities directly from a browser without programming in JAVA.

Whereas the original plan was for specific, qualified module developers to each develop a module per year, Etomica permits modules to be assembled by any faculty member and students to investigate molecular simulations in general. In essence this development environment takes the place of many of the originally proposed modules. However, we are using Etomica also to assemble several standard, pre-prepared modules. Using Etomica, a developer pulls in pieces of the simulation applet including simulation essentials (types of molecules to use, types of interactions, type of integrator, type of boundary conditions, simulation box, etc.), a user interface (temperature slider, composition slider, time step box, control buttons, etc.), and an output interface (meters to monitor desired properties such as strip chart recorders, graphs, text boxes, tables, etc.). The developer then must set up the web pages to display the applet and provide the student and instructor materials.

During the past year we have added additional output meters and considerably revised some of the features and the code to eliminate bugs and facilitate its use. Etomica now constitutes a unique platform for development of molecular simulation tools. Etomica has been tested at State University of New York, Buffalo, by high school students who have designed their own simulations using Etomica. Additionally, we have used Etomica to develop several modules, and these modules are being tested in the classroom and by other members of the committee. These modules have been targeted at specific undergraduate courses in accord with the original objectives of the project. Course supplemental materials including instructor materials, student problems, and tutorials have been developed and launched with these modules. Assessment information for the developed modules has been developed and implemented. A web page has been established from which the web modules can be obtained by course instructors. A standard format has been developed for the instructional materials so that the user interface is comfortable and useable from one module to the next. Information about the developed modules have been conveyed in national meetings and a set of papers to appear in *Chemical Engineering Education* are currently in the review process.

An itemization of the results are:

1. Revision and Completion of Etomica. Available for developers from:
   http://www.ccr.buffalo.edu/etomica/

2. Module web page from which completed modules can be obtained:
   http://www.et.byu.edu/~rowley/WebModules/modules.htm

3. Two summer workshop courses for high school students with 9 applets developed using Etomica. See
   http://wings.buffalo.edu/eng/ce/kofke/applets/

4. Over 10 different applets developed using Etomica. For a list of these, see
   http://wings.buffalo.edu/eng/ce/kofke/applets/

5. Completed modules with instructional material now available from the link listed in item 2.
   a. **Title:** Multicomponent Phase Equilibrium
      Purpose: Molecular simulations are used to elucidate the concept of chemical potential in multicomponent systems, and how the chemical potential relates to multicomponent phase equilibrium.
      Applicable Classes: Thermodynamics
      Author: Daniel Lacks
      Affiliation: Tulane University

   b. **Title:** Vapor Liquid Equilibria
      Purpose: Provide a molecular visualization of the equilibrium vapor and liquid phases corresponding to real binary mixtures. Students at any level in their curriculum can get a better feel for the relationship between the

interactions between molecules and the resultant extent of the phases (mass balances) and the equilibrium compositions (equality of component chemical potentials).
Applicable Classes: Separations, Material and Energy Balances, Thermodynamics
Author: Richard Rowley
Affiliation: Brigham Young University

c. **Title:** Molecular Aspects of Thermal Conductivity
Purpose: Using an interactive simulation applet, the module attempts to strengthen the link between traditional macroscopic engineering approaches to heat transfer and the concepts from kinetic theory that students learn in physical chemistry courses. Students will learn what properties influence the ability of different materials to conduct energy, as well as how the transport coefficients can be calculated from knowledge of the molecular-level structure and energetics of the material.
Applicable Classes: Heat Transfer, Fundamentals of Transport Phenomena, Molecular Modeling
Author: Randall Snurr
Affiliation: Northwestern University

d. **Title:** Joule-Thomson Effect
Purpose: In this module, you will investigate the Joule-Thomson effect, using classical thermodynamics along with molecular simulation. You will explore how the relationship between temperature, pressure and intermolecular forces leads to a given temperature change upon expansion. At the completion of the module, you should be able to answer Joule and Thomson's question!
Applicable Classes: Thermodynamics
Author: Edward Maginn
Affiliation: Notre Dame University.

5. Publications/Presentations on this Work During this Period of Time

a. Four presentations on this project and module work were given at the national AIChE meeting in Reno, NV, November, 2001.
b. Invited submission to *Chemical Engineering Education* for the four papers presented at the above meeting.

6. Implementation of Module Assessment. Modules are assessed as they are used by the students and feedback is sent to the PIs so that the modules can be improved. This also allows us to assess learning and achieved objectives from the modules. How the modules are utilized and their effectiveness can be correlated to student learning styles. See:
http://ntmis.cc.nd.edu/chemeng/CHEMENG.SURVEY_MENU.show