

## **IOWA STATE UNIVERSITY**

A new Web site has been created that shows a collection of thermodynamic fundamental and state surfaces for generic one-, two-, and three-component, fluid-phase systems as modeled by the Peng-Robinson equation using common mixing rules. Kenneth Jolls (Iowa State University) and Daniel Coy (Nanophase Technologies Corporation) have used high-performance computer graphics to produce three-dimensional, parametric sections of the n-dimensional fundamental functions that result from various Legendre transformations. Selected equation-of-state surfaces resulting from differentiation of the fundamental forms are shown also and their connections with the parent functions are noted. Each surface covers a property range spanning a fluid-phase critical point, and color is used to partition the functions according to thermodynamic stability theory. The presentation offers excellent collateral reading for any advanced treatment of theoretical classical thermodynamics, such as in the books by Modell and Tester (Reid) or by Callen. The Web site has the title "Gibbs Models" and can be viewed at:

[www.public.iastate.edu/~jolls/](http://www.public.iastate.edu/~jolls/)

## **IOWA STATE UNIVERSITY/RICE UNIVERSITY**

A computer based tutorial for thermodynamic phase diagrams of binary, ternary, and quaternary systems has been developed at Iowa State University under the direction of Ken Jolls and at Rice University under the direction of Walter G. Chapman. The tutorial allows students to view, rotate, and slice 3-D phase diagrams interactively on a PC. The tutorial is a combination of powerpoint presentation and C++ visualization programs. For example, the student can view of P-T-xy diagram for a binary system and make constant temperature or constant pressure slices through the diagram. This enables the student more clearly see the form of the bubble and dew surfaces. The tutorial is available from Walter G. Chapman at Rice University by filling out the form on the web site:

[www.owlnet.rice.edu/~wgchap](http://www.owlnet.rice.edu/~wgchap).

The program uses the Open Inventor graphics library which was licensed from Silicon Graphics. Chapman has purchased a large number of licenses so that one copy is available to each university. Additional copies of the tutorial are available at the nominal cost of \$20 per copy. The tutorial provides an excellent introduction to thermodynamic phase diagrams for undergraduate and graduate students.

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## **LEHIGH UNIVERSITY**

We have recently released a set of ODE/DAE/PDE applications in the following areas:

1. Mass transfer and separations
2. Reactors and kinetics
3. Heat transfer
4. Fluid flow
5. Process control

Details for obtaining this set of applications are given in:

<http://www.lehigh.edu/~wes1/wes1.html>

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## **MANHATTAN COLLEGE**

1. Puri, Welsh and Chickos. Integrated computational and experimental investigation of the thermodynamic properties of polychlorinated biphenyls. University of Missouri.
2. Bamford. The prediction of Henry's law constants and its temperature dependence for polychlorinated biphenyls from computational and experimental data. Chesapeake Biological Laboratory, University of Maryland.
3. Totten, Liu, Braun and Assaf-Anid. Success of density functional theory in predicting enthalpy changes associated with two-electron reduction of polychlorinated biphenyls. Rutgers University, Columbia University and Manhattan College.
4. Fransisco. Atmospheric chemistry of alternative fuels. Purdue University
5. Tossell. Computing the properties of the Cu-thioarsenite complex. University of Maryland.

Please check our website:

<http://www.engineering.manhattan.edu/chemical/news/-events.html>