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Solving Chemical Equilibrium Problems Online

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Requires Java applet compatible Web browser

A Java web application, or "applet", has been developed to assist chemistry educators, students, and researchers in solving general multiphase chemical equilibrium problems involving many species. Analysis of chemical equilibria is a topic frequently covered in both undergraduate and graduate courses in physical chemistry, chemical thermodynamics, and engineering thermodynamics. In such courses, manual calculations of problems that require a student to solve for species concentrations or mole fractions usually involve the use of equilibrium constants. Exercises in homework assignments and classroom examinations are frequently limited to reactions that involve no more than four gas-phase species, as the resulting arithmetic required to solve for unknown molar quantities becomes too cumbersome and prone to error. When manually solving equilibrium problems in homework assignments, students need a tool to verify their answers. Furthermore, educators and researchers who encounter complex chemical equilibrium problems require access to a software package that will allow one to define a multiphase, multicomponent reactant mixture and compute not only the equilibrium distribution but also the thermodynamic state of the equilibrium mixture.

The applet presented in this article is an easy-to-access and simple-to-use application that allows one to rapidly define the composition and thermodynamic state of a reactant mixture, compute the equilibrium distribution, and view the product composition and state using an intuitive graphical user interface. Several examples are presented on how our Java applet can be used by educators to enhance the curriculum in their courses. A complete and rigorous overview of the numerical method implemented within the applet, based on the nonlinear constrained minimization of the product mixture Gibbs function, is also given. A discussion of how an object-oriented approach was used in the design of the classes used to build the applet is presented. A UML diagram is also presented showing the relationships among the classes used to implement the applet's composition panel, which is used to define reactant and product mixtures (Figure 1).

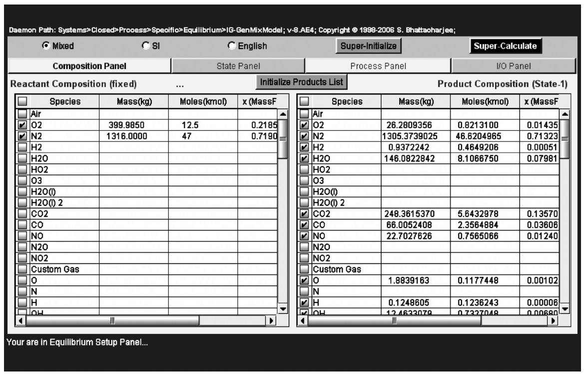

Figure 1. Results of using the applet to calculate the equilibrium distribution of octane for $\phi = 1$ (combustion of isooctane and air for $\phi = 1$ at $p = 50$ bar and $T = 3000$ K).

The applet was first used in a production capacity in fall 2008 when it was introduced as part of the curriculum in a thermodynamics course. A survey was conducted afterward to evaluate student experience using the tool and informally measure how use of the applet contributed to an overall understanding of chemical equilibrium concepts presented in class. Results of this survey are presented along with several examples including a complex combustion reaction involving isooctane and air.

Supporting Information Available

Expanded article; Java Web application; survey results. This material is available via the Internet at http://pubs.acs.org.

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