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Solving Chemical Equilibrium Problems Online

Christopher Paolini* and Subrata Bhattacharjee

College of Engineering, San Diego State University, San Diego, California 92182-1326 *paolini@engineering.sdsu.edu

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

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

€ Mixed C SI		C English State Panel Initialize Pr			Super-initialize Process Panel Products List Pr		Super-Calculate ### ### ### ### ####################		
Composition Panel									
Reactant Composition (fixed)				Pro					
	Species	Mass(kg)	Moles(kmol)	x (MassF		Species	Mass(kg)	Moles(kmol)	x (MassF
	Air			_		Air			
	02	399.9850	12.5	0.2185		02	26.2809356	0.8213100	0.01435
	N2	1316.0000	47	0.7190		N2	1305.3739025	46.6204965	0.71323
	H2					H2	0.9372242	0.4649206	0.00051
	H20			1	×	H20	146.0822842	8.1066750	0.07981
	H02					H02			
	03					03			
	H2O(I)					H2O(I)			
	H2O() 2					H2O(I) 2			
	C02					C02	248.3615370	5.6432978	0.13570
	CO					co	66.0052408	2.3564884	0.03608
	NO					NO	22.7027626	0.7565066	0.01240
	N20				HE.	N2O	22.7027020	0.1303000	0.01240
	NO2			_	ΗE	NO2			
	Custom Gas			_	H	Custom Gas	_		
		-		_	15	O Custom Gas	1.8839163	0.1177448	0.00102
							1.0038103	0.1177440	0.00102
				_	H	N			
	H					H	0.1248605	0.1236243	0.00006
1	1114			1	14	III III	12.4633079	111/2/1/048	0.00680

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).

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).

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.