A Cyber-based Collaborative Framework for Thermodynamic Education and Research

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For last ten years, we have been building a comprehensive webware TEST – The Expert System for Thermodynamics, accessible from www.thermofluids.net - for thermodynamic education and practice. TEST is a visual platform where a user can look up traditional charts and tables, visualize thermodynamic systems through animations and interactive dynamic images, browse thermodynamic problems and solutions enriched with multimedia, and employ web-based thermodynamic calculators called *daemons* to solve most traditional thermodynamic problems on topics ranging from energy, entropy and exergy analysis of generic systems to analysis of air-conditioning or combustion applications. Once a visual solution is obtained, the solution can be used as a baseline case for a myriad of parametric studies or what-if scenarios. Created with web friendly tools, TEST is platform independent, can be locally installed for speed, and is completely browser based. A TEST solution - although visual in nature - can be saved, recreated instantly, or shared through email for remote collaboration.

In this presentation, we will demonstrate some of the features of TEST through its combustion and chemical equilibrium daemons. Using this as the basis, we will introduce our future plan that can be quite relevant to the combustion community. We would like to develop the existing webware into a community based suite of tools that can be enriched by users, allowing them the ability to prototype new chemical structures and upload thermochemical specifications to a shared, Internet accessible database. New species would be tagged as experimental and then be assigned different confidence levels after passing a peer-reviewed vetting process. New species added to the database are made immediately available to all researchers in real-time for use in constructing reactant mixture compositions or in the specification of product compositions when performing an equilibrium analysis. The initial database will be populated with thermochemical data adopted from the NIST WebBook (http://webbook.nist.gov/). Our solvers will run Java Web Service (WS) and will be made available to the Internet grid computing community. Developers of distributed and grid enabled combustion applications will be free to invoke the resources of our chemical equilibrium web service on demand. Communication to and from our web service is encapsulated in an XML framework. Each equilibrium problem will be specified in XML and passed by the developer's client application to our web service for computation. The solution will then be calculated by our web service and passed back to the client as an XML message encapsulating the moles or masses of each product species. Our web service will run in a standard open source servlet container such as Apache Tomcat (http://tomcat.apache.org/) and be implemented using a standard open source SOAP engine such as Apache Axis (http://ws.apache.org/axis/). We envision our implementation of a chemical equilibrium web service will amount to a plug-and-play computational software environment, freely available to developers of cyber-based combustion applications. Researchers and educators would be able to outsource most of their equilibrium computational needs to this web-based service and couple these remote procedure calls in their existing or future computational codes.