

Process Informatics

Investigator: David M. Golden, Professor, Mechanical Engineering

"PrIME" (Process Informatics Model) is a community activity aimed at the development of predictive reaction models for combustion. The primary motivation is to establish and demonstrate the community approach to kinetic-model development and, perhaps most importantly, establish a means for reaching community consensus on the models and data.

The initial objective is the creation of the PrIME library.

The PrIME project originated from informal discussions held during the 77th International Bunsen Meeting of Deutsche Bunsen-Gesellschaft für Physikalische Chemie on "Formation and Degradation of Hydrocarbons in High-Temperature Reactions," Bad Herrenalb, Germany, October 7-11, 2001. A position paper was prepared that summarizes the underlying ideas. These ideas were proposed to GCEP with the following schedule and checkpoints:

- (1) By July 1, 2004 _____ evaluate and compile reaction and thermochemical parameters in the initial combustion mechanism.
- (2) By July 1, 2003 _____ prepare a report that outlines the work needed and the funding required to proceed with the development and implementation of *Process Informatics*.

The position paper that summarizes the underlying ideas and philosophy of the project is *attached*. Although GCEP funding was not yet in place, an informal meeting of interested researchers was held on July 22, 2002, during the 29th International Symposium on Combustion, Sapporo, Japan and a report of this meeting was prepared and is available on request.

Current activities underway include:

- Creation of the PrIME team and its organization into PrIME working groups.
- Creation of the PrIME Library and associated activities to evaluate and compile reaction and thermochemical parameters in the initial combustion mechanism.

A web site for the project, with much background and planning information is available at <http://purl.oclc.org/NET/prime/>

Contact:

D. Golden: david.golden@stanford.edu