

Process informatics for chemical reaction systems

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The present frontier of combustion chemistry is the development of *predictive* reaction models, namely, chemical kinetics models capable of accurate numerical predictions with quantifiable uncertainties. While the usual factors like deficient knowledge of reaction pathways and insufficient accuracy of individual measurements and/or theoretical calculations impede progress, the key obstacle is the inconsistency of accumulating data and proliferating reaction mechanisms. *Process Informatics* (aka PrIME for Process Informatics Model) introduces a new paradigm: a one, community-maintained “ever-green database”, and on-the-fly-generated models (rather than “mechanisms”) produced to answer specific questions.

Process Informatics is a data-centric approach and deals with all aspects of integration of pertinent data of complex systems (industrial processes and natural phenomena) whose complexity originates from chemical reaction networks. It relies on three major components: proper organization of scientific data, availability of scientific tools for analysis and processing of these data, and engagement of the entire scientific community in the data collection and analysis. The proper infrastructure will enable a new form of scientific method by considering the entire content of information available, assessing and assuring mutual scientific consistency of the data, rigorously assessing data uncertainty, identifying problems with the available data, evaluating model predictability, suggesting new experimental and theoretical work with the highest possible impact, reaching community consensus, and merging the assembled data into new knowledge and predictive models.

As of this writing, PrIME is a “grass-roots” initiative (<http://primekinetics.org>), with various activities/parts funded by NSF-ITR, NSF Cyberinfrastructure, and DOE-MICS-CMCS programs. The PrIME infrastructure has two principal components: a Data Warehouse (<http://primekinetics.org/warehouse>; User Name = “prime_guest”, Password = “prime_guest”; a simple search portal is activated by clicking on “search.asp”) and a collection of Tools. The Warehouse is designed to represent the most currently complete set of knowledge available in a given field. The currently built Tools are of two general kinds, those enabling the collection, transfer, organization, display, curation, and mining of the data, and those enabling processing and analysis of the data along with assembly of the data into models.

The list of PrIME activists and contributors currently includes M. Frenklach, Z.M. Djuricic, A. Packard (UC Berkeley); D.M. Golden, C.T. Bowman (Stanford); W.H. Green, G.J. McRae (MIT); P.J. Smith, A.F. Sarofim (Univ. of Utah); T.C. Allison, W. Tsang (NIST); J. Frey, M.J. Pilling (UK); B. Ruscic (ANL); H. Wang (USC), P.R. Westmoreland (Univ. of Mass.); V.D. Knyasev (Catholic U.); N.J. Brown (LBL); G.P. Smith (SRI); K. Brezinsky (Univ. of Illinois at Chicago), ... and the list is growing. The PrIME Initiative will be launched on April 21-22, 2006.