Process Informatics Model (PrIMe): A Systematic Approach to Building Combustion Chemistry Models

Investigators
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Abstract

This project has seen the development of Process Informatics in the form of PrIMe, move from a concept to a reality. The funding herein was largely used to inform the community of the power of the PrIMe ideas. As this is written, data is being transformed into XML format and stored on servers. The public release of the database is about one month away. New funding was obtained from NSF Chemistry for cyberinfrastructure development and a now a workshop on the subject has been scheduled at NSF by combustion related sections. A major presentation will be made at the International Symposium on Combustion in Heidelberg this August.

Introduction

Development of new energy-efficient low-emitting combustion technologies requires models for the combustion process that combine sub-models for combustion chemistry, heat and mass transfer, and fluid mechanics. A major limitation in developing these process models is the availability of accurate, validated, and computational tractable combustion chemistry models. This research is aimed at the development of a new approach for constructing and reducing models of complex chemical reactions. It has been termed *Process Informatics.* This endeavor is made possible by recent advances in computer science that allow assembly and manipulation of large amounts of data that may be scattered over different sources using Web-based computer networks. The goal is to convert combustion chemistry model building into science, to automate the methodology, and to make the information available in a prompt and convenient form on the Internet for researchers and designers of combustion equipment

Background

A good deal of the effort in this particular project is in essence political. That is, it involves community organization in the combustion research community and it requires the acceptance of a somewhat different paradigm than the standard in the community. External developments in the field in the past several years involve several workshops and symposia in which the PrIMe idea has continued to gain currency. Presentations by the PI, Professor Golden, as well as American collaborators at UC Berkeley, MIT, SRI International and international collaborators from the UK and the Continent and other such developments are discussed below in the “Results” section of this report.

It was previously reported that The National Institute of Standards and Technology (NIST) had agreed to be the permanent host for the PrIMe Library and eventually for the computer based tools required for model development. Since that time, it has been decided that the servers needed will be hosted by the CITRIS (Center for Information Technology research in the Interest of Society: http://www.citris.berkeley.edu/) project at UC Berkeley. Some of these tools are being developed in a Sandia National laboratory

led effort called, Collaboratory for Multi-scale Chemical Science (CMCS). Initially PrIMe will be available at Sandia as well. Professor Golden is a member of the Advisory Board of CMCS. Interest in industry is also picking up.

In 2005, the National Science Foundation issued a solicitation entitled: Chemistry Research Instrumentation and Facilities: Cyberinfrastructure and Research Facilities. The program to "provide funding to build a foundation for cyber-enabled chemical research and education". A proposal encompassing PrIMe was submitted as a collaboration between Stanford, (Golden), UC Berkeley (Frenklach and Packer) and MIT(McRae and Green). The proposal was accepted and has been funded. Work is ongoing at all three instutions.

This solicitation grew, from among other events, a report on cyberinfrastructure discussed in the NSF solicitation. "As described in the report, "Revolutionizing Science and Engineering Through Cyberinfrastructure: Report of the NSF Blue-Ribbon Advisory Panel on Cyberinfrastructure," the manner in which scientific and engineering research and education is conducted will be radically transformed by cyberinfrastructure. This report may be accessed at http://www.cise.nsf.gov/sci/reports/atkins.pdf. The NSF Division of Chemistry shares this vision and has held a workshop that has identified research and education frontiers that would be enabled by investments in cyberinfrastructure. The report from this workshop may be accessed at http://bioeng.berkeley.edu/faculty/cyber_workshop/. A National Research Council report, "Information and Communications," also identifies opportunities in cyberinfrastructure in the chemical sciences and is available at http://books.nap.edu/catalog/10831.html."

Results

The first goal of the PrIMe project is the creation of a database or library, sometimes referred to as a warehouse for combustion data. The goal is an agreed upon, evaluated by the community, updated in a timely fashion, data library. The library is open, accessible to all and contains, beside the agreed upon values, all data and all dissents from the consensus evaluation. There are some models for this type of activity, Professor Golden has been a member of the NASA/JPL Panel that evaluates rate data for atmospheric modeling, but the goal here is more far-reaching. All background information used in the evaluations will be available.

This program requires bringing a large community together and it has been somewhat slower than hoped, but is now close to realization. Professor Golden, Professor Michael Frenklach of the University of California, Berkeley and Professor Michael Pilling of Leeds University have acted as a "troika" in engaging the community. Prominent additions to the active team include Dr. Wing Tsang of NIST, Professors William Green and Gregory McRae of MIT and Dr. Jeremy Frey of The University of Southampton, UK. Many other workers have expressed their willingness to participate.

The first informal gathering of possible PrIMe participants took place during the International symposium on Combustion in Sapporo, Japan in August 2002.

Professor Frenklach of UC Berkeley made a presentation at the DOE Basic Energy Sciences Contractor's Meeting in Lake Tahoe, CA in May 2003 that outlined possibilities associated with this project. He and colleagues have published an article[1] in December 2003 that points out the large amount of information available from extant experiments that is not being accessed as result of lack of familiarity with many statistical procedures that can now be accomplished with relative ease. A second article[2] by the Berkeley group on mutual consistency of data appeared recently.

A meeting at NIST in September 2003 aimed at establishing a data base for "Real Fuels" served as a venue for discussions that resulted in NIST becoming a key player in PrIMe. At that meeting Professor Golden explained the procedures used to develop the widely used Natural Gas combustion mechanism, known as GRI-Mech. He pointed out all the ways this could be better accomplished once PrIMe is underway. Professor Frenklach, once again described the future of process modeling.

In March 2004 there was a symposium in the Fuel Section of the National American Chemical Society Meeting in Annaheim , CA. Two days of speakers discussed combustion modeling and PrIMe was a central focus in several presentations. (The agenda is attached and those presentations directly involving PrIMe related activities are highlighted.) A presentation based on collaboration with Professor William Lester, Professor Frenklach and students at UC Berkeley, includes Professor Golden. A paper based on this presentation has been published[4] in the International Journal of Chemical Kinetics, and is listed below.

In October 2004, there was a meeting at NIST during which the PrIMe concepts were briefed to a group of government Program managers. The briefing was conducted by Professors Golden, McRae and Frenklach and Dr. J. Manion of NIST. Program managers present were: Frank Tully, Dick Hilderbrandt and Eric Rohlfing all of DOE, Julian tishkoff of AFOSR, David Mann of ARO and Linda Blevins of DOE. A copy of the informal review of that meeting is attached.

At this time all the background data used in developing the GRI-Mech model has been cast into XML format and the very large amount of data available at Leeds University will be translated and made available for PrIMe. Extensive data searching tools are also being developed.

Dr. Gregory P. Smith of SRI International, Menlo Park, CA has together with Professor Frenklach and colleagues at Berkeley, applied the tools of process informatics to understanding a dichotomy in the understanding of OH chemistry in the upper stratosphere and the lower mesosphere. A paper[3] has been submitted.

In July 2005 the International Conference on Chemical Kinetics was held at NIST. Professor Frenklach gave an invited talk that was an overview of the PrIMe process.

Conclusions

In past instructions for GCEP reports we were asked to provide a discussion of the progress achieved to date toward the goal of developing the basis for technology options that could lead to substantial reductions in emissions of greenhouse gases that result from energy use. In other words, describe the potential impact of the research, if successful, on greenhouse gas emissions at a global scale.

This is a far-reaching goal. The goal is to make modeling and design of combustion driven devices easier and accurate, with the goal of energy efficiency and minimal pollution of all kinds. Engineering advances require the ability to make models of practical processes. PrIMe is designed with this in mind.

This research project was really the tip of an iceberg. There will be ongoing work in codification of data in XML format and in putting together the evaluation teams. There will be an ongoing attempt to secure funding for a large scale collaborative effort. The work put into the effort to secure NSF support did bear fruit. We have put together a team and documentation for further attempts to secure funding. Unfortunately even the modest support for Professor Golden that would have allowed his continued participation was not forthcoming from GCEP.

Publications and Presentations

1. Evaluating and Codifying Data for Engineering Applications
   Presented by David M. Golden at NIST Workshop on Real Fuels, September 2003

2. Quantum Monte Carlo study of the thermochemistry of small hydrocarbons
   Kollias, A., Domin, D., Frenklach, M., Golden, D.M., and Lester, W. A., Jr.
   Accepted for publication International Journal of Chemical Kinetics

3. Presentation by David M. Golden at NIST briefing October 2004.

References

1. Frenklach, M. , Packard, A., Seiler, P., and Feeley, R.,; Collaborative data processing in developing predictive models of complex reaction systems, Int. J. Chem . Kinetics 2004, 36, 57-66

2. Feely, R., Seiler, P., Packard, A., and Frenklach, M.,; Consistency of a reaction dataset, J. Phys. Chem. A 2004, 108, 9573-9583.

3. Smith, G. P., Frenklach, M. , Packard, A., Seiler, P., and Feeley, R. A System Analysis Approach for Atmospheric Observations and Models: the Mesospheric HOx Dilemma,

4. Kollias, A.C., et al., Quantum Monte Carlo study of heats of formation and bond dissociation energies of small hydrocarbons. International Journal of Chemical Kinetics, 2005. 37, 583.

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