

Combustion Simulation Databases for Real Transportation Fuels: A New Community Collaboration

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The economic, environmental, and health benefits that could be derived from improved combustion processes are enormous and well recognized. In September 2003, the leading experts from industry, academia, and government met at the NIST Workshop on Combustion Simulation Databases for Real Transportation Fuels to assess needs and opportunities to translate scientific understanding of combustion to technological development. Attendees affirmed the value of predictive models of combustion in the development of less polluting engines. The workshop concluded that a coherent effort is required to address the complexities associated with the combustion of real transportation fuels and that a standard infrastructure for the exchange of combustion-related data must be developed.

As a result of the workshop, NIST joined with other members of the combustion community in the PrIME (Process Informatics Model) collaboration. The goal of PrIME is to generate standard formats for combustion data, together with data libraries, analysis software tools, and the supporting IT infrastructure that will enable development of predictive models for combustion. The PrIME uses the DoE supported (CMCS) project to develop and support the IT infrastructure required for the effort. NIST's commitment to PrIME envisions the creation of new paradigms for scientific collaboration involving the construction of a traceable, comprehensive electronic repository of key data relevant to modeling combustion processes.

The initial data library consists of data from the NIST Chemical Kinetics Database and GRI-Mech 3.0 (the current "standard" model for combustion of small hydrocarbons). The library includes data collections on atomic properties, chemical species, thermodynamics, elementary kinetics, and transport, as well as bibliographic data. A collaborative workspace for the PrIME project has been created within the CMCS portal.

Ultimately the PrIME project will facilitate the rapid construction of predictive models for combustion chemistry.

Launching of the initial PrIME data repository is anticipated in the first half of 2005. Longer-term plans include the integration of sophisticated tools that reduce human efforts in model creation and reduction.

NIST/CSTL leads the creation of a standard infrastructure for the exchange of combustion data, which is critical to technological development.

<http://kinetics.nist.gov/RealFuels/>

