

The following two items are an outcome of the discussion held on July 22, 2002, during the 29<sup>th</sup> International Symposium on Combustion, Sapporo, Japan:

- A. There is clear consensus for moving ahead with a community activity for development of reaction models of combustion.
- B. There is wide consensus on taking methane combustion as the “show case” system. While there still exist problems with specific details of methane kinetics, the primary motivation for choosing this system is to establish and demonstrate the community approach to kinetic-model development and, perhaps most importantly, establish a mechanism for reaching community consensus on the models and data.

For implementation of this initiative, we propose the following guiding principles and concrete initial steps.

#### **GUIDING PRINCIPLES:**

- I. *Open Membership*—Any scientist can be part of this initiative.
- II. *Open Source*—All data and models “submitted” to the project or created by the project will become “public domain”, following the paradigm of the Open Source Initiative for software development (<http://www.opensource.org/>); the precise definition(s) and the license to be worked out as part of this initiative.
- III. *Democratic Governance*—The project management will follow rotational leadership guided by community consensus; the specifics to be worked out as part of the initiative.

#### **INITIAL STEPS:**

1. *Collection of pertinent kinetic and experimental data on methane combustion kinetics*—Everyone is invited to “submit” his or her species thermodynamics, reaction rate coefficients, and experimental observations pertinent to the methane combustion system. The key point of this “submission” process is conversion of the data files into an XML file format. (A very brief description of XML is given in Appendix A.) With data coded as XML files will allow complete and reliable automation of data exchange, archival of scientific information, and minimization of errors associated with data transfer.
2. *Creation of a community web site for the project*—All communication among the team participants, developers and users, will be facilitated by a modern-technology web site. We will start a web site (current plan is it will be hosted at the Combustion Research Facility in collaboration with Larry Rahn) enabled by tools from the CMCS project as they become available (see Appendix B). Such a site is being “prepared” as you read this document, and everyone will be notified of its availability soon (we plan on it by the end of August). The site will contain all further information, including how to join the group, how to submit the data, how to access the data, along with suggested XML formats and converters.

**PRESENT STATUS AND ACTION ITEMS:**

- a) The GRI-Mech 3.0 dataset is now being transformed into XML format as part of CMCS activities. These data, explanation of their organization, and associated templates will be made available through the PrIME web site (PrIME portal).
- b) Mike Pilling and Peter Glarborg indicated they would follow with their reaction data sets. Bill Pitz has already translated LNLL reaction mechanisms into XML format. Charlie Westbrook, Fred Dryer, and Wing Tsang, among others, expressed their enthusiasm for the initiative.
- c) *Initiative Name*—We need a name to identify the project. The name we started with is PrIME, for **Process Informatics Model**. Is this acceptable? Do you have other suggestions?
- d) *XML Data File Location*—There are, in principle, two choices. One is to physically place all XML files on a single server. CMCS offers us space on their WebDAV server along with their developed tools (file management, XML translators, search engines, and the like). This would allow us to start the project immediately, with every contributor having its own, clearly identifiable domain, and to use powerful searching, storing, and retrieving capabilities that are becoming available. The second option, of XML files distributed among various servers, while also in the CMCS vision, is not yet available. Do you have any preference on this matter?

**APPENDIX A: XML Format**

XML stands for “Extensible Markup Language”. We presume that you have some rudimentary knowledge of HTML. XML is similar to HTML in that it is also a (plain) ASCII file, but differs from it primarily in that you can make your own tags. The idea is that every piece of information is tagged. This allows easier, more flexible, and essentially universal storage, retrieval, and exchange of data than probably any other form. Once the data is placed into an XML file, you do not need to retype it ever again—an XML file can be “easily” parsed (read) and translated (converted) into any other format; here is where CMCS tools come into play. The XML syntax is stricter than HTML: XML is case sensitive and requires a closing tag. The main challenge is in organization of data into separate XML “compartments”, files, and collections (directories). The following is an example of an XML file for the definition of a chemical species:

```
<?xml version="1.0" ?>
<molecule id="c2h4">
  <nomenclature>
    <name type="CAS">74-85-1</name>
    <name type="formula">C2H4</name>
    <name>ethene</name>
    <name>ethylene</name>
  </nomenclature>
  <composition>
    <chemElement id="C">2</chemElement>
    <chemElement id="H">4</chemElement>
  </composition>
</molecule>
```

**APPENDIX B: CMCS Project**

CMCS stands for “Collaboratory for Multi-scale Chemical Sciences” (<http://cmcs.ca.sandia.gov>), a project of the SciDAC (Scientific Discovery through Advanced Computing; <http://www.scidac.org/>) initiative of the U.S. Department of Energy. CMCS is a collaboration of computer scientists and scientists from eight U.S. laboratories and universities. One of the objectives of CMCS is to “facilitate scientific collaboration by providing project/community management tools relevant to researchers that are integrated with the public CMCS data and capabilities”. CMCS expressed an interest in using the PrIME project as their pilot; in turn, the PrIME community can benefit immediately from the CMCS services and tools.