May 30, 2017

Dear Bonnie Lawlor, Chair of the Committee on Publications and Cheminformatics Data Standards:

Last month we submitted a proposal entitled “*ThermoML 2017—Revision of an XML based IUPAC Standard for Thermodynamic Property Data*”. We wanted to provide you with responses to the comments of the Internal and external IUPAC reveiwers.

Most of the input agreed that it is a legitimate proposal, and it matches the goals and strategic thrusts of IUPAC as well. The members are from multiple communities and represent experts in their fields. The

From the comments, we saw four main issues:

1. That there was confusion about the requested funding
2. Broadening the dissemination plan / increasing community awareness
3. Development of commercial and open-source tools & modular framework
4. Support of ThermoML

***In response to funding:***

NIST is providing the funding for the development of the software related to ThermomL: An updater so that older thermoML files can be converted to the new format, and a generic reader for users to view the data in a human readable format or in machine readable format. This funding is through the Materials Genome Initiative and base funding from NIST.

The requested amount 14k is to pay for the travel of members on the committee to the meetings, as many of the members cannot self-fund their travels. We assume this will pay for the lodging and a plane ticket for 3-4 committee members, to large thermophysical property conferences, that could not make It otherwise to ECTP in Gratz, Austria and STP, in Boulder, CO, USA.

We can ask for funding from other sources if necessary as indicated by reviewer e(V) comment 7.

***In response to broadening the dissemination plan:***

The suggestions of providing professional society publishing houses with information on the progress of the project (the AWS, TMS, JOM ) can definitely improve the breadth and commentary that we get from data users.

This can and will be added to the dissemination plan.

***In response to development of open source and commercial software, tools and modular framework:***

The development of commercial tools is outside of the scope of this update--while our group at NIST does provided commercial software to this effect, this development is out of scope from updating ThermoML. The standard is already in commercial use with software companies, with the ThermoML Updater all commercial users will be able to update their old files and use the new software or have a means for backwards compatibility.

We hope during the commentary phase commercial data users will give us input to missing fields or attributes required by their industries to be incorporated into the standard. We have worked with industrial partners for the adaptation of ThermoML in the past. We see this update as a modernization of the XML too which in later forms could help support commercial software.

We are aiming to work with other communities including the Materials Genome Initiative to help support modular schema development. First we wanted to develop the backbone (provenance, processing, systems, phase characterization) to which modules could be added for future applications (even those outside of the organic and metallurgical communities) of materials science.

***In response to support of ThermoML:***

It was mentioned that: “ *The ThermoML webpage is, at the moment, better available from the NIST webpage than from IUPAC webpage. It is a joint effort involving several international organizations besides IUPAC, which must be supported*.”

NIST is glad to maintain and provide the proposed dictionary, and namespace for the schema as done in the past. We are willing to work with other organizations to provide simple-single representation for ease of use, while maintaining the needs and changes required through communication with other organizations.

With the proposed changes:

1. Expanding dissemination plan to include short briefs to JOM and Welding Journal
   1. This should also help with the industrial/commercial software interfacing necessary for the ThermoML expansion
2. Indicate support from NIST for software development in funding section

Please let us know if there are any further concerns, or anything else we need to address.

Regards,

Boris Wilthan

Erik Pfeif