

Thermo SIG Progress Report 2011 and Future Outlook

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Thermodynamics Special Interest Group (Thermo SIG)

Task:

Develop, maintain and promote Thermodynamic and Physical Properties interface specifications

Key Responsibilities:

- ◆ **Maintain and manage existing interface specifications**
- ◆ **Assess expansions of interface specifications**
- ◆ **Manage the development of expansions**
- ◆ **Help organizations to develop implementations**

Thermo SIG Members, September 2012

- ◆ Alan Scott, contractor for TÜV-SÜD-NEL
- ◆ Andrew Lintern, HTRI
- ◆ Bjorn Maribo-Mogensen, Technical University of Denmark
- ◆ Ensheng Zhao, Honeywell
- ◆ Jasper van Baten, AmsterCHEM (SIG co-leader)
- ◆ Michel Pons, CO-LaN
- ◆ Murugesh Palanisamy, Honeywell
- ◆ Paul Zhou, Honeywell
- ◆ Rafael Lugo, IFP
- ◆ Richard Szczepanski, Infochem Computer Services
- ◆ Sergej Blagov, BASF (SIG co-leader)
- ◆ Suphat Watanisiri, AspenTech
- ◆ Xiaozheng-Sara Wang, Honeywell

Thermo SIG Accomplishments 2011

◆ Interface specification documents

- Revised documents published
 - Thermodynamic and Physical Properties** interface specification v1.0 & v1.1
- New Errata and Clarification documents started
- Revision on-going
 - Chemical Reactions** interface specification
(add to **Thermodynamic and Physical Properties** interface specification v1.1)
- Proposal under discussion
 - Compound Server** interface specification

◆ Help to developers

- Open Source Examples of **Property Package** & **Property Package Manager** (v1.1) and **ThermoSystem** (v1.0)

◆ Phone meetings and Lotus Quickr Team Place

Errata & Clarifications Documents

- ◆ **Thermodynamic Standard specification 1.1 (version 3.11)**
 - Minor changes
 - Mainly tips for effective implementation and usage (SetMaterial, bubble and dew point calculation, surface tension, etc.)
 - Update to be published in October, 2012, after approval in SIG Thermo
- ◆ **Thermodynamic Standard specification 1.0 (version 1.08.008)**
 - Many tips for effective implementation and usage (naming of phases, error codes, heat of vaporization, etc.)
 - Important clarification / correction concerning CalcType for pressure and temperature
 - Update to be published prompt in October, 2012, after approval in SIG Thermo
 - New revision (1.08.009) required; RFC to be started in 2012

Chemical Reactions Interface

- ◆ **Several issues exist with current v1.0 Reactions specification**
 - Reaction basis is not clearly defined
 - Units of measure require revision (non-SI)
 - Several concepts not well defined
- ◆ **Large overlap with v1.1 Thermodynamic and Physical Properties**
 - Compound definitions
 - Material contexts
- ◆ **Conclusions:**
 - Need for a new **Reactions** interface specification
 - Need for integration with v1.1 **Thermodynamic and Physical Properties** interface specification
- ◆ **Status:**
 - Revision done; RFC starts in October, 2012

Chemical Reactions Interface: Key Features

◆ Generality in focus

- Different phases might be specified for reactants and products on component basis
- Various reaction types
 - Single phase reactions
 - Interfacial and Surface reactions
 - Homogeneous and Heterogeneous reactions
- Formulation on the true species basis

◆ Very compact

- Only 4 reaction properties supported
 - Reaction rate
 - Chemical Equilibrium Deviation function
 - Chemical Equilibrium Deviation tolerance (constant value)
 - Enthalpy of Reaction

Compound Server Interface Proposal

- ◆ **Existing CAPE-OPEN PPDB interface is complex**
 - Very wide scope
 - Not targeted at delivering single recommended values
- ◆ **Need for pure compound server delivering**
 - Compound constants
 - Compound correlation descriptor
 - Compound correlation coefficients
- ◆ **Current proposal: no support for mixture model data**
 - Too complex
 - Models not always uniquely defined
 - Model coefficients may depend on other models
- ◆ **Status**
 - Draft version of simplified interfaces applicable for both v1.0 and v1.1 thermodynamic component specifications prepared
 - No much interest so far
 - Decision required !

Examples of Thermodynamic Components

- ◆ CO-LaN contracted AmsterCHEM
- ◆ Ideal Mixture Thermodynamics Library as an example
- ◆ Full Implementation
 - Property Package & Property Package Manager (v1.1)
 - ThermoServer (v1.0)
- ◆ C++ and VB6 versions
- ◆ ‘How to’ implementation
- ◆ Clarity is focus; no optimization for performance
- ◆ Open source published

Feedback on Examples

- ◆ Used to test and report problems in existing PME
- ◆ **BASF adaptation experience**
 - C++ version
 - No skills in **ATL/COM** programming
 - 2 weeks demand for ~ 1/3 of all v1.1 interfaces
 - Most time – adjustment of the native thermo-library
 - Still complex for inexperienced program developer
 - Requires ‘step-by-step’ guidelines
- ◆ **More feedback needed !**

Summary

- ◆ **Thermo v1.0 & v1.1: applicability proven**
- ◆ **Thermo specifications maintenance**
 - **Relies successfully on Thermo SIG**
- ◆ **Looking forward to more and further usage**
 - **New extension interfaces under discussion**
 - Reactions interface
 - Compound server interface
 - **Round-table Thermo SIG session here, September, 20th, 15:00-17:00**

Questions?

Thank you for your attention!



Go CAPE-OPEN!