

Thermo SIG Progress Report 2010 and future outlook

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Thermodynamic Special Interest Group (Thermo SIG)

Task:

Develop, maintain and promote Thermodynamic and Physical Properties interface specifications

11 members from 8 companies

Key Responsibilities:

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

Accomplishments 2010 & Main Deliverables 2011

Thermodynamic and Physical Properties interface specification

- Revision completed for both v1.0 & v1.1
- Includes "Errata & Clarifications" recorded in the past
- No impact on formal interface definitions

New Interfaces to add

- **Chemical Reactions** interface specification
- **Compound Server** interface specification

Help to developers

- Open Source Examples of Implementation

➔ new specification documents available from

<http://www.colan.org>

➔ under discussion

see 'Thermo SIG'-flyer for details

➔ feedback needed; source code available from

<http://www.colan.org/News/Y11/news-1125.htm>

Perceptions of CAPE OPEN are not always right

Conflicting statements about CO-Thermodynamics:

- too slow vs. too complex

Complexity of CO-Thermodynamics results from the requirements for

- high flexibility and high performance

Ways to reduce the perceived complexity

- Detailed step-by-step guidelines
- Further investigations needed
- Simplified 'Thermo'-Wizard/Template with built-in COM-support ?
- New CAPE-OPEN **Object Model** without COM (**Methods and Tools SIG**) ?

Performance issue is problem of implementation and not of specification

BASF performance tests for several thermodynamic packages

Simulator:	Thermodynamic Package			
	Native BASF Thermo-Library	BASF EOS-Library via ForeignObject interface by gProms	CO compliant Multiflash via	
<i>Chemasim</i> 12 comp. mixture PSRK-NRTL ~ 100 eq. stages			general: FORTRAN- Thermo-Wrapper (ProSim)	specialized: BASF- AmsterCHEM Material Object
Performance: CPU-time, s	1.01	12.94	8.55	1.86

Specialized Material Object

- High performance compared to EOS-Library or Thermo-Wrapper
- Good acceptance by end users; growing number of users
- High potential for further performance improvements (e.g., batch calculation of properties in a single call)

Thermo SIG Challenges

Thermo v1.0 & v1.1: applicability proven

Thermo specifications maintenance

- Relies successfully on Thermo SIG

CO Thermo interfaces are working well

- Let this be better known!

Increase acceptance by academics and small companies

Accelerate migration from v1.0 to more powerful and better structured v1.1

