

Thermo SIG Progress Report 2023

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Thermo SIG Annual Report: Charter

Scope:

- Thermodynamics and Physical Properties interface specification v1.0 (deprecated)
- Thermodynamics and Physical Properties interface specification v1.1 (active)
- Custom Data interface specification v1.1 (active)
- Chemical Reactions interface specification v1.1 (pending Manager)
- Compound Server interface specification (on hold)

and related documents, files, tools, software, and procedures.

Thermo SIG Annual Report: Charter

Key Responsibilities:

- ❑ Maintain and manage active interface specifications (revisions to improve design, performance/speed and robustness based on user input)
 - Provide errata and clarifications and integrate in current specification
- ❑ Assess and prioritize on expansions of thermodynamic interface specifications
- ❑ Help CO-LaN members to develop implementations of thermodynamic interfaces
 - Provide advice on migrating from deprecated to active interface versions
 - Provide advice on new implementations
 - Analyze interoperability issues between PME and PMCs
- ❑ Define compliancy tests for thermodynamic interface specifications

Thermo SIG Annual Report: Membership

- Sergej Blagov
- Jasper van Baten
- Klaus Möller
- Michel Pons
- Richard Szczepanski
- Bjørn Maribo-Mogensen
- BASF (co-leader)
- AmsterCHEM (co-leader)
- University of Cape Town
- CO-LaN
- KBC Advanced Technologies Ltd
- Hafnium Labs

Summary of activities 2022-2023

- ❑ **Specification document for a Manager Common Interface**
 - **Draft was finalized**
 - **Handed draft over to Methods & Tools SIG**

- ❑ **Thermodynamics and Physical Properties interface specification v1.1**
 - **Specification of tests**
 - **Errata & Clarifications**
 - **Laborious (as expected)**

Custom Data interface specification

- ❑ Published in November 2019
- ❑ Currently known implementations:
 - PME: COFE (AmsterCHEM)
 - PMC: ProTreat Thermo (Optimized Gas Treating)
- ❑ Thermo SIG recommends developing support in PMEs
 - Implementing support in a PME is not much work.
 - Required to support revised Chemical Reaction interface specification.
 - May become mandatory on Material Object in future versions of CAPE-OPEN standard.

Chemical Reactions interface specification

- ❑ **M&T SIG needs to submit Manager Common interface specification for RFC.**
- ❑ **Upon publication of Manager Common interface specification, references will be incorporated into revised Chemical Reactions interface specification.**
- ❑ **At this point, revised Chemical Reactions interface specification will be ready for a second RFC.**

Certification support

□ Specification of tests

- Current focus is on Property Package testing as a PMC
- Learning curve: UNIT Operation PMC, PME thermodynamic socket, PME unit socket

	Thermo	Unit
PMC under test	<p>Test Engine PME</p> <ul style="list-style-type: none">• controls thermodynamic calls• validates thermodynamic provider (Property Package)• <i>provides Material Object</i>	<p>Test Engine PME</p> <ul style="list-style-type: none">• receives thermodynamic calls• validates correctness of thermodynamic calls• <i>provides Material Object</i>
PME under test	<p>Test PMC (Property Package)</p> <ul style="list-style-type: none">• receives thermodynamic calls• validates correctness of thermodynamic calls• <i>validates Material Object services (storage, basis conversion,...)</i>	<p>Test PMC (Unit Operation)</p> <ul style="list-style-type: none">• controls thermodynamic calls• validates thermodynamic provider (PME/Material Object)• <i>validates Material Object services (storage, basis conversion,...)</i>

Certification support

❑ Validating the testability of published interface specification

- Any requirement should be testable

❑ Errata & Clarifications

- No major issue requiring immediate release of new version of specification
 - This was expected on basis of 20+ years of interoperability
- Large number of clarifications identified when preparing tests
 - What is not explicitly stated cannot be tested
 - E&C to be submitted for RFC (much work expected from reviewers)
 - E&C to be integrated in revision of interface specification (for readability)
- Mostly clarifications but some changes made to CAPE-OPEN contract

Errata and Clarifications: strategy

❑ Callee/caller responsibilities

- **Current specification leads often to implementations with validity of arguments checked by both caller and callee: makes tests impossible to design**
 - If caller (test) does not respect contract, callee behavior is undefined
- **Clarification of responsibilities (callee/caller)**
 - **Examples:**
 - Caller cannot guess Phase labels or Compound identifiers
 - Physical Property identifiers are in general pre-defined (standardized)
- **The same responsibility must sit on one side only**
 - “You must do that” avoids “you must check that it is like that”
 - Property Package does not need to check Phase labels used as input arguments when there is no ambiguity (e.g., only one Phase supported)
 - **Caller must use only phase labels supported by the Property Package**

❑ Working implementations override specifications

- **20+ years of interoperability gives basis for interpretation of unclear points**

Errata and Clarifications: major changes

❑ Unclear/too implicit requirements

▪ Example

- All methods cannot raise “Not implemented” exception
- For methods returning lists of identifiers, returning UNDEFINED (empty list) is valid
 - Not supporting anything is not an error, it is valid

❑ Phase presence: whole new chapter written

❑ Consistency of capabilities between methods

- *GetSinglePhasePropList*, *CheckSinglePhasePropSpec* and *CalcSinglePhaseProp*
- *GetTwoPhasePropList*, *CheckTwoPhasePropSpec* and *CalcTwoPhaseProp*
- *CalcAndGetLnPhi* and *CalcSinglePhaseProp*

Errata and Clarifications: major changes

- ❑ **Material Object responsibilities made explicit:**
 - **Basis conversion**
 - **Inter-conversion between flows and fraction, on overall and on phases**
- ❑ **May derive properties not available from original source (e.g., using basic thermodynamic relationships):**
 - **If Property Package provides density but not volume, Material Object may provide volume out of density.**
 - **The same may go for derivative properties or any derived properties.**
- ❑ **Clarification on static information**
 - **Static information does not depend on Material Context**

Test of Property Package as a PMC

- ❑ 72 tests implemented so far:
 - *ICapeIdentification (specified by M&T SIG)*
 - ICapeThermoCompounds
 - ICapeThermoMaterialContext
 - ICapeThermoPhases
 - ICapeThermoUniversalConstants

- ❑ Specification underway – not yet implemented
 - ICapeThermoPropertyRoutine
 - ICapeThermoEquilibriumRoutine

□ Work outlined for this year:

■ Support

• Certification:

- define the remaining tests for Property Package PMC testing
- start work on PME and Unit PMC testing

• Maintain and manage existing interface specifications

■ Publish Chemical Reactions interface specification

- Reference Manager Common interface specification
- Launch RFC, publish IDL, disseminate

Questions?

Thank you for your attention!



Go CAPE-OPEN!