Thermo SIG Progress Report 2024

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Thermo SIG Membership

- Sergej Blagov
- Jasper van Baten
- Klaus Möller
- Kyle Abrahams
- Richard Szczepanski

- BASF (co-leader)
- AmsterCHEM (co-leader)
- University of Cape Town
- CO-LaN
- KBC Advanced Technologies Ltd

Thermo SIG Charter: Scope

- ~~Thermodynamics and Physical Properties interface specification COM v1.0 (deprecated)~~
- Thermodynamics and Physical Properties interface specification COM v1.1 (active)
- Thermodynamics and Physical Properties interface specification COBIA v1.2 (unpublished but in production)
- Custom Data interface specification v1.1 (active) (+v1.2)
- Chemical Reactions interface specification v1.1 (+v1.2)
- Compound Server interface specification?

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

Thermo SIG Charter: Key Responsibilities

- Maintain and manage active interface specifications
  - Provide revisions to improve design, performance and robustness
  - Provide errata and clarifications and integrate in specifications
- Assess and prioritize on extending specifications
- Help CO-LaN members to develop implementations of thermodynamic interfaces
  - Provide advice to software developers
    - on migration to newest interface specifications
    - on migration from COM to COBIA
    - on new implementations
  - Analyze interoperability issues between PME and PMCs
- Define compliancy tests for thermodynamic interface specifications

Deprecation of v1.0

- Deprecated per December 31, 2017
- Discussed at the CAPE-OPEN 2017 Annual Meeting
- CO-LaN no longer supports this specification.
- There will be no update of the specification document.
- There will be no additional Errata & Clarifications
- CO-LaN is encouraging all software developments to use version 1.1+ interface specification.
- Consequently: we removed it from our charter.
- CAPE-OPEN 1.0 TLB will remain part of the CAPE-OPEN 1.1 type library installer

Summary of activities 2023-2024

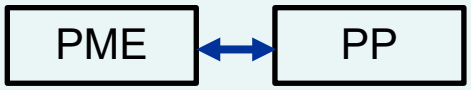
- **Thermodynamics and Physical Properties v1.1**
  - **Completion of Chemical Reaction Interface specification**
  - **Specification of tests**
    - **Completed Property Package PMC testing specification**
      - **Except Common Interfaces → M&T SIG responsibility**
    - **Completed Material Object specification of Unit PMC testing**
  - **Errata & Clarifications**
    - **Numerous issues clarified → Extensive document set**
    - **Revised interface and method descriptions for nearly all Thermodynamic interfaces**

Chemical Reactions interface specification

- Manager Common interface specification is published
  - Interface specification available from CO-LaN web site
  - IDL in preparation: COBIA route (COBIA presentation)
- References are incorporated into revised Chemical Reactions interface specification: use cases updated
- Chemical Reactions interface specification is submitted for a second RFC
- Release strategy (to do):
  - Publish Specification Document on CO-LaN web site
  - IDL: COBIA route (COBIA presentation)

Certification support: 1

- **Active thermodynamic interface testing:**
  - **Collection of Test Specifications**
  - **Go hand-in-hand with Errata and Clarifications**



	Thermo	Unit
PMC under test	Test Engine PME • controls thermodynamic calls • validates thermodynamic provider (Property Package) • *provides Material Object*	Test Engine PME • receives thermodynamic calls • validates correctness of thermodynamic calls • *provides Material Object*
PME under test	Test PMC (Property Package) • receives thermodynamic calls • validates correctness of thermodynamic calls • *validates Material Object services (storage, basis conversion,…)*	Test PMC (Unit Operation) • controls thermodynamic calls • validates thermodynamic provider (PME/Material Object) • *validates Material Object services (storage, basis conversion,…)*

Certification support: 2

- Property Package PMC Testing was initial focus (Test suite beta release)
- Unit PME Testing: very similar; unit can actively exercise thermodynamics
  - But: thermodynamics implemented by Material Object, fixed component slate
  - Not yet on release path

	Thermo	Unit
PMC under test	Test Engine PME • controls thermodynamic calls • validates thermodynamic provider (Property Package) • *provides Material Object*	Test Engine PME • [illegible]ives thermodynamic calls • val[illegible]rrectness of thermody[illegible]lls • *provides Materia[illegible]*
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Minor modifications

Certification support: 3

- **Unit PMC Testing**
  - **Opposite traffic: thermodynamics interface gets exercised**
  - **Requirement on the Material Object: detect incorrect calls only**
  - **Material Object implementation specifications delivered**

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Certification support: 4

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Minor modifications

E&C: release strategy

- E&C cannot be released without RFC
  - RFC modifications may be challenged by community
- Test suite and E&C are interdependent
  - E&C are adapted to ensure testability of standard
  - Tests depend extensively on new E&C Documentation
- Test suite beta goes hand-in-hand with E&C RFC
  - Separate presentation by Malcolm Woodman
- Integration of E&C into main document postponed:
  - Prerequisite: Common Source CAPE-OPEN Documentation
  - Separate presentation by Kyle Abrahams

Compound Server Component: 1

History

- Physical Properties Data Bases Interface: too complex
- CAPE-OPEN 1.1 offers ICapeThermoCompounds
  - Sufficient for pure compound information
  - No functional description
  - No validity range on T- (and P-) dependent properties
  - No mixture data (binary interaction coefficients)
- Honeywell expressed interest in a simpler design, around 2008
- Thermo SIG drafted initial “Compound Database Component” specification, 2011
  - Compound Server: ICapeThermoCompounds implementation
  - Compound Correlation Server: as above + correlations with coefficients and range
  - No mixture data: deemed not useful due to dependence on specific models
- Honeywell was no longer actively participating, so proposal was shelved

Compound Server Component: 2

❑ Recent discussions

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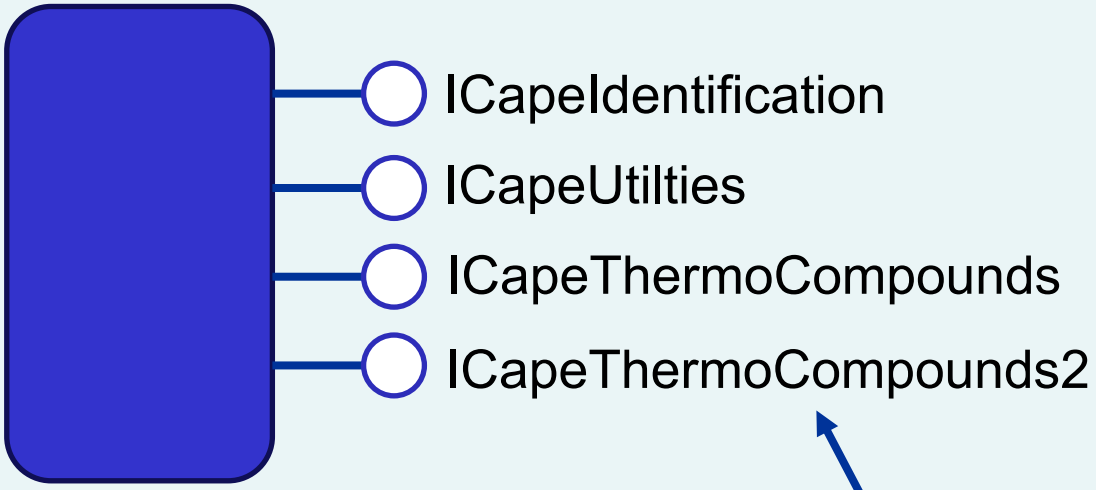
Compound Server Component: 3

❑ Revised proposal



Compound Server Component: 4

- **Future:**
  - **Is there an interest in the community to follow-up?**
  - **Should Thermo SIG:**
    - **Make a revised and simplified proposal?**

      or

    - **Drop this from the Charter?**

Outlook 2024-2025

- Work outlined for coming year:
  - Support
    - Provide feedback for certification implementations
    - Maintain and manage existing interface specifications
  - Publish Chemical Reactions interface specification and IDL
  - Design structure for Common Source CAPE-OPEN Document
  - Integration of E&C documentation

Questions?

Thank you for your attention!

Go CAPE-OPEN!

Backup

E&C: some changes in 2024

- Common
  - Clarification on when errors are valid
  - Clarification on which methods are mandatory
  - Clarification on present phases and phase status
  - Expected behavior on unphysical values (e.g., negative T)
  - Clarifications on basis conversions
- Property Routine
  - Supported Properties must be calculatable at some condition
  - Clarifications on missing and partial values
  - Absent compounds and present compounds with zero (mole-) fraction should yield same result
  - Clarification on phase order for TwoPhase properties
- Equilibrium Routine
  - If CalcEquilibrium fails, state of Material Object is undefined