Thermo SIG Progress Report 2014

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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 2014

- **Andrew Lintern,** **HTRI**
- **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 Activities 2013-2014

- **Efforts concentrated on finalizing the Chemical Reactions interface specification v1.1**
  - Main ideas first presented on CO-LaN Annual Meeting, 2012, Lyon, France
  - Second revision presented on CO-LaN Annual Meeting, 2013, Lyon, France
- **Ongoing work in a small group**
  - Jasper van Baten, Michel Pons, Sergej Blagov
  - 2 hours weekly remote desktop sessions
- **Still not finished**
  - Main problem:

    How to deal with “equilibrium” reactions in a general way?

Chemical Reactions Interface v1.1: Motivation

- **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
- **CO-LaN Annual Meeting, 2012, Lyon, France:**
  - First draft presented
  - Major drawbacks recognized:
    - Formulation on the true species basis
    - Not well suited for polymers, electrolytes, etc.
    - No reactive phase equilibrium calculator defined

Chemical Reactions Interface: Key Features

- **Generality**
  - Different phases might be specified for reactants and products on component basis
  - Various reaction types (single phase, interfacial, homo/hetero-geneous, etc.)
- **Compactness**
  - Only 4 reaction properties supported
    - Reaction Rate
    - Chemical Equilibrium Deviation
    - Chemical Equilibrium Deviation tolerance
    - Enthalpy of Reaction
- **Flexibility**
  - Multiple Compound Slates (for different sets of apparent compounds)
  - Material Object Delegates in addition to Material Object

Chemical Reactions Interface: v1.1 vs. v1.0

- Integration with the CAPE-OPEN version 1.1 thermodynamic standard, as opposed to ‘stand-alone’ interface
- This eliminates the redundant definitions for compounds
- Units of measure are SI (as opposed to version 1.0)
- Reactions can be served by Property Package, or by Reaction Package

Chemical Reactions Interface: v1.1 vs. v1.0

- **Material Object manages its Material Object Delegates associated with appropriate Compound Slates**
- **Reaction Object discarded, this task is to be performed by the Material Object**
- **Reaction Context discarded**
  - for Reaction servers this is the Material Context
  - a Unit Operation can obtain reactions ONLY from an associated Material Object (e.g. connected stream)

Chemical Reactions Interface: v1.1 vs. v1.0

- ***Equilibrium constant*** **discarded in favour of** ***EquilibriumDeviation***
- **Reaction phase replaced by vector: one phase for each compound (e.g. solid C can react with gaseous O2)**
- **Reaction rate basis (reaction domain):** ***Phase***, ***PhaseInterface***, ***CatalystMass***, ***Surface***
- **Both** ***ReactionRate*** **(stoichiometry required) and** ***CompoundReactionRate*** **(stoichiometry is optional) are supported**

Chemical Reactions Interface. New in v1.1

- **Reaction attributes:** ***Mechanism***, ***Kinetic***, ***Equilibrium***, ***Comment***, ***Catalyst***, ***FullConversion,*** *etc.*
- **Equilibrium reaction sets:** sets of equilibrium reactions that need to be considered simultaneously
- **Overall pseudo-kinetic reaction:** several kinetic reactions lumped into one, for which only per-compound reaction rates are provided
- **Reaction groups:** optional arrangement of related reactions, for aiding reaction selections in private GUIs
- **Reaction alternatives:** multiple versions of the ‘same’ reaction with different properties, e.g., rate expression

Chemical Reactions Interface. True & Apparent

Example

A + B == C

Systems 1/3 A + 2/3 B and 1/2 B + 1/2 C are equivalent

Glossary

- ***Apparent compounds***
  - A set of Apparent compounds is any set of compounds that allows for unique specification of equilibrium state of a mixture (here: {**A,B**}, {**A,C**}, {**B,C**})
- ***True compound***
  - Any compound which may eventually appear at equilibrium (here: **A**, **B**, **C**)
- ***Compound Slate***
  - Any collection of Compounds allowing for representation of a given system
- ***Compound Server***
  - Implements *ICapeThermoCompounds*; serves as source for compounds definitions
- ***Material Object Delegate***
  - … is an alternative representation of the Material Object for a particular Compound Slate

Chemical Reactions Interface. True & Apparent

- Compound Server might expose multiple Compound Slates
- *ICapeThermoCompounds* operates on a particular Compound Slate
- There exists the default (Master) Compound Slate (not necessarily the *True* one)
- Compounds can be *True*, *Apparent* or both
- Associated equilibrium calculation is reactive
- Equilibrium calculation operates on a Material Object Delegate
- States of Material Object and all its Material Object Delegates are synchronized
- Conversion between apparent composition and *True* composition done by Property Package (optional)
- Support for *Apparent* properties (e.g. fugacity)

Chemical Reactions Interface. Equilibrium Calculations

- **Performed by Equilibrium Servers**
  - Implement ***ICape…EquilibriumRoutines***
  - **Material Objects**, **Property Packages** and **Equilibrium Calculators**
- **Principal difference for reactive and non-reactive systems as**
  - for reactive systems, overall compositions and total mole numbers are calculation results and not constants

Equilibrium server / Interface	Conventional (non-reactive)	Reactive
ICapeThermo-EquilibriumRoutine	mandatory	mandatory (throws error)
ICapeThermo-ReactiveEquilibriumRoutine	optional (same results)	mandatory

Summary

- Thermo v1.0 and 1.1 specifications maintenance
  - Sustainable usage
  - Very few issues for clarification reported
  - v1.0: significant overhead both for support (CO-LaN) and development
    - Time to deprecate? => presentation by Michel Pons
- In focus: Chemical Reaction Interface Specification v1.1
  - Major revision of draft document was required
  - Ongoing work on a new draft

    (weekly phone meetings: J. van Baten, M. Pons, S. Blagov)
  - Goal:
    - present the final draft on CO-LaN Annual Meeting, 2015

Questions?

Thank you for your attention!

Go CAPE-OPEN!