Thermo SIG Progress Report 2013

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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 2013

- **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**

Chemical Reactions Interface (September 2012)

- **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/November, 2012**

Chemical Reactions Interface: Key Features (September 2012)

- **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

Finalizing of Chemical Reactions Interface

October / November, 2012

- **Preparation of the finalized version of Chemical Reaction Interface started (J. van Baten, M. Pons, S. Blagov)**
- **Major drawbacks recognized (mainly feedback from M. Pons):**

- True species approach does not allow for hiding any details of reaction mechanism
- Stoichiometry must always be explicitly defined and exposed
- No means provided for handling systems of special type, e.g. polymers, electrolytes, etc.
- Reactive phase equilibrium calculator not defined, which is, however, of most interest for users

- **Major revision required**

Chemical Reactions Interface Specification. I

Comparison of revised 1.1 Reactions interface to existing 1.0

- 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 Specification. II

Comparison of revised 1.1 Reactions interface to existing 1.0

- 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 Specification. III

Comparison of revised 1.1 Reactions interface to existing 1.0

- ***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** ***Reaction Rate*** **(stoichiometry required) and** ***CompoundReactionRate*** **(stoichiometry is optional) are supported**

Chemical Reactions Interface Specification. IV

New in version 1.1 specification

- **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 Specification. V

Reactive Phase Equilibrium Calculator

- A reaction for which the overall equilibrium composition is part of the result
- No Reaction Package needed
- Performed by Equilibrium Server (e.g. Property Package or native PME thermo)
- Requires new interface: *ICapeThermoReactiveEquilibrium*
- *True* composition is separately stored on Material Object
- *MolarReactionRatio* - an additional output argument:

$$= \frac{\text{Total mole number AFTER}}{\text{Total mole number BEFORE}}$$

Chemical Reactions Interface Specification. VI

True vs *Apparent* Compounds

- *ICapeThermoCompounds* exposes union of *True* and *Apparent* compounds
- Compounds can be *True*, *Apparent* or both
- Associated equilibrium calculation is reactive
- Equilibrium calculation operates with *True* compounds only
- State of Material Object is defined by pressure, temperature and *True* composition
- Conversion between apparent composition and *True* composition done by Property Package (if provided)
- Support for *Apparent* properties (e.g. fugacity)

Summary

- Thermo v1.0 and 1.1 specifications maintenance
  - Sustainable usage
  - Very few issues for clarification reported

    - v1.0: CalcType for P & T: both, 'Mixture' and UNDEFINED are to be allowed

- In focus: Chemical Reaction Interface Specification
  - Major revision of draft document was required
  - Ongoing work on a new draft

    (weekly phone meetings: J. van Baten, M. Pons, S. Blagov)
  - Deadline still not fixed

    (for some concepts there is no standard solution and they need further elaboration)

Questions?

Thank you for your attention!

Go CAPE-OPEN!