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,
- Andrew Lintern,
- Bjorn Maribo-Mogensen,
- Ensheng Zhao,
- Jasper van Baten,
- Michel Pons,
- Murugesh Palanisamy,
- Paul Zhou,
- Rafael Lugo,
- Richard Szczepanski,
- Sergej Blagov,
- Suphat Watanisiri,
- Xiaozheng-Sara Wang,

contractor for **TÜV-SÜD-NEL** HTRI **Technical University of Denmark** Honeywell **AmsterCHEM** (SIG co-leader) CO-LaN Honeywell Honeywell IFP **Infochem Computer Services BASF** (SIG co-leader) AspenTech 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

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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

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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

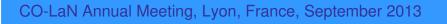
Comparison of revised 1.1 Reactions interface to existing 1.0

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:

Total mole number AFTER

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 <u>True</u> 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-OPENI

CO-LaN Annual Meeting, Lyon, France, September 2013

