Thermo SIG Progress Report 2019

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Thermo SIG Annual Report: Charter

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 Annual Report: Membership

- Sergej Blagov — BASF (co-leader)
- Michel Pons — CO-LaN
- Mark Stijnman — Shell Global Solutions
- Jasper van Baten — AmsterCHEM (co-leader)
- Ryan Liu — Honeywell Process Solutions
- Bjørn Maribo-Mogensen — Hafnium Labs
- Richard Szczepanski — KBC Advanced Technologies Ltd
- Suphat Watanasiri — Aspen Technology, Inc.
- Jian Yong (Jim) Yang — Honeywell Process Solutions

Summary of activities 2018-2019

- Errata Thermo 1.1
  - Diffusion coefficients and more
  - RFC finished December 2018: few responses
  - Ready for public release pending MB approval
- Material Template System
  - Several issues identified with current System
  - New System proposed to M&T SIG

Summary of activities 2018-2019

- Custom Data interface specification
  - RFC finished December 2018: many comments received. Thanks!
  - Modifications made in response to comments
  - Ready for public release pending MB approval
- Chemical Reactions interface specification v1.1
  - Finalized heat of reaction, introduced Reduced Reaction set
  - Ready for RFC except for revision of Manager Common Interface

Goals set for 2019: comparison with expected

- **RFC initiated for Custom Data** done
  - **Analysis of comments** done

- **RFC for Reactions**
  - **Need to complete heat of reaction issues** done
  - **Unforeseen work:**
    - **Reduced Reaction Set** done
    - **Develop a common Manager interface (e.g. for Property Package Managers): still on-going**

Errata Thermo & Physical Properties 1.1

- As discussed at CAPE-OPEN 2018 Annual Meeting
- Three new properties:
  - diffusionCoefficientAtInfiniteDilution: $D_{i,j,x_j \to 1}$
  - diffusionCoefficientMaxwellStefan: $Đ_{i,j}$
  - diffusionThermodynamicFactor: $\Gamma_{i,j} = \delta_{i,j} + x_i \left. \frac{\partial \ln \gamma_i}{\partial x_j} \right|_{T,P,x_{k,k \neq j}}$
- Ambiguous property ‘diffusionCoefficient’ deprecated
- Comments received through RFC are positive

Clarifications Thermo & Physical Properties 1.1

Additional clarifications:

(see E&C document for details)

- **Phase Attribute**
- **Phase Identification**
- **Phase Consistency at Phase Equilibrium**
- **Continuity of Phase Properties**
- **Behaviour Expected From Material Object during CalcEquilibrium**
- **Phase Status**
- **Surface Tension**
- **Naming of Material Objects**
- **Re-establishing Connection Between PME and Property Package**
- **Number of Values Returned and Order**

Issues with Material Template System

- Problem of scoping / responsibility
  - *ICapeThermoMaterialTemplate* belongs to THRM
  - *ICapeMaterialTemplateSystem* belongs to COSE

- Problem with *ICapeThermoMaterialTemplate*
  - *SetProp(property, values)*: what does it mean?
  - Only one other function: *CreateMaterialObject*
  - No need to create an object for creating an object

New interface proposal

- *ICapeThermoMaterialTemplate* + *ICapeMaterialTemplateSystem* = ***ICapeThermoMaterialTemplates***
  - **Better name?**
  - **Belongs to THRM**
- **Two members:**
  - **Property *MaterialTemplateList* as CapeArrayString**
  - **CapeInterface *CreateMaterialObject*(templateName)**
- **Proposed to M&T SIG in February 2019**
  - **Names modified since this proposal**
- **Thermo SIG recommends use of new interface in COBIA**

Custom Data

- **Custom Data summary:**
  - **Allows storage of PMC's specific data on Material Object**
    - **Custom Data Container is the per-Material-Object storage**
    - **Custom Data Source is the PMC that stores the data**
  - **A means to improve performance of chemical equilibrium calculation**

- **Modification following RFC:**
  - **Custom Data Source notified of thermodynamic configuration changes**
  - **More efficient than discarding/re-creating Custom Data Containers**

Reaction interface: Heat Balance

- **Generic approach introduced**

$$\Delta h_r^{exp} = \frac{Q}{\Delta\xi} = \frac{(N^* + \Delta\xi * \Sigma\nu_i) * h(T^*, P^*, \mathbf{n}^* + \Delta\xi * \boldsymbol{\nu}) - N^* * h(T^*, P^*, \mathbf{n}^*)}{\Delta\xi}$$

$\Delta\xi \to 0$

$$\Delta h_r = (\Sigma\nu_i) * h(T^*, P^*, \mathbf{n}^*) + \Sigma\nu_i * \frac{\partial h}{\partial n_i}(T^*, P^*, \mathbf{n}^*)$$

known to CRS

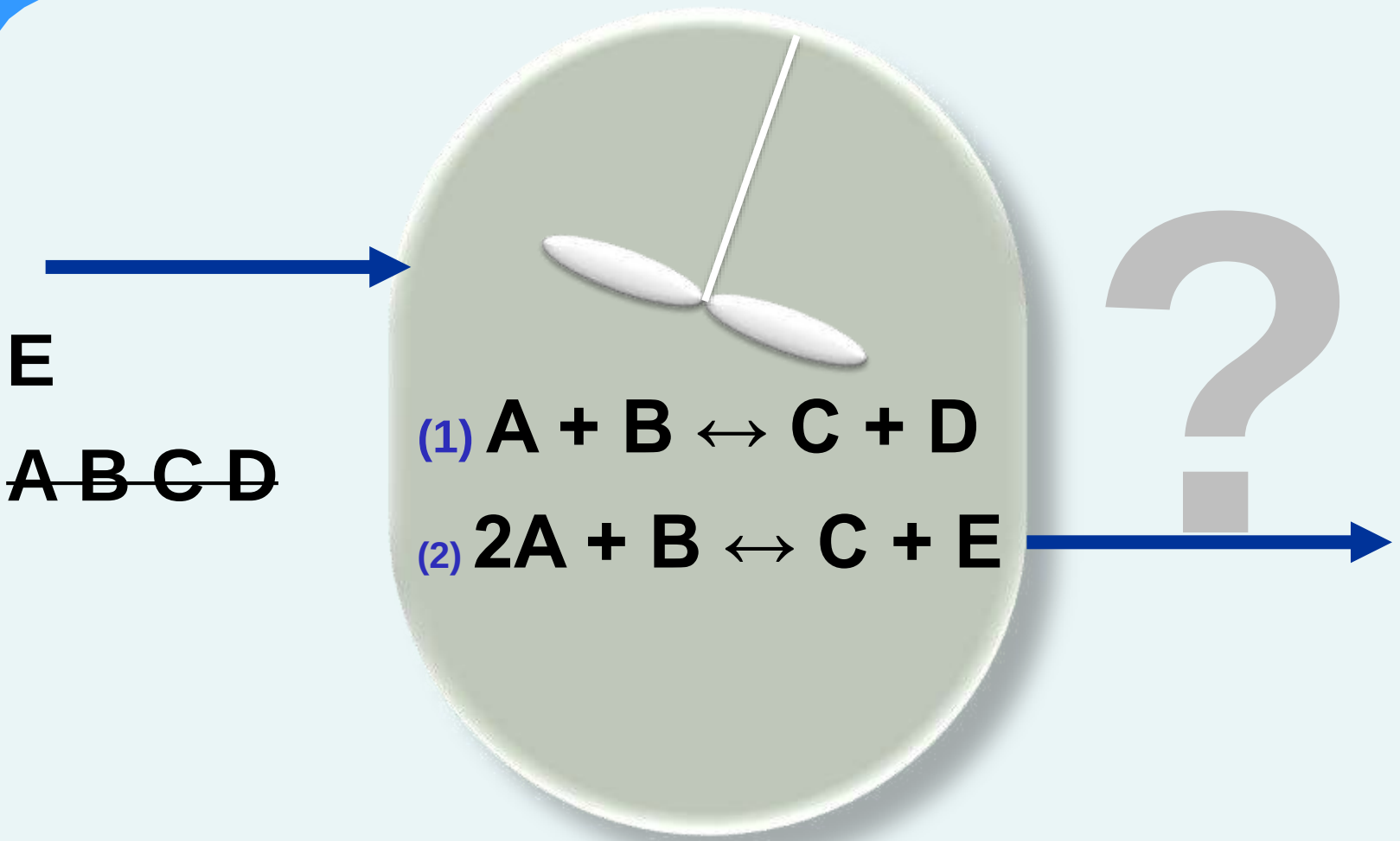
done

using Property Package

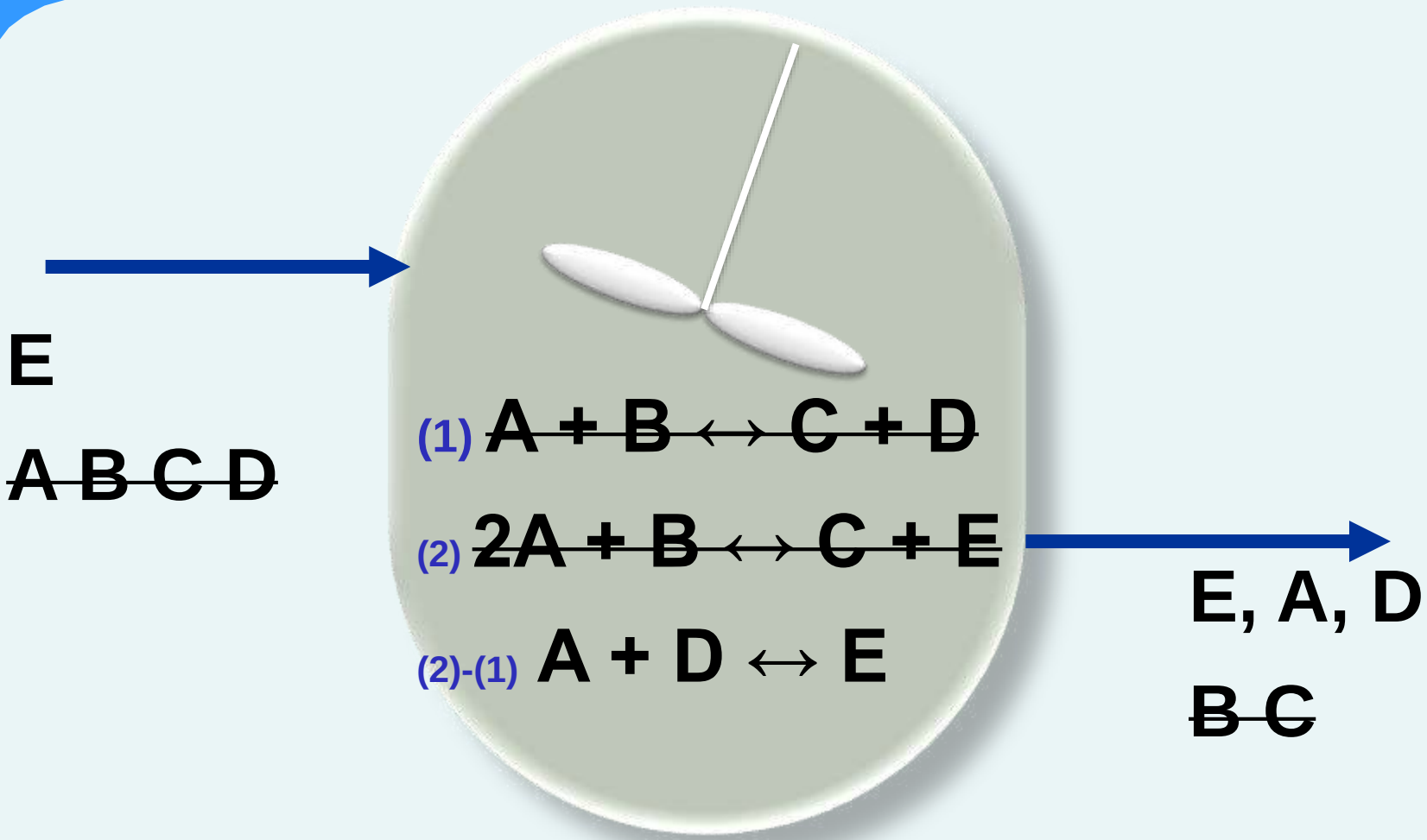
$$\Delta h_{\mathrm{BCOR}} = \Delta h_r^{exp} - \Delta h_r(T^*, P^*, \mathbf{n}^*)$$ – constant, to be calculated once

- **Reaction Server: *enthalpyBalanceCorrectionOfReaction***
- **Several examples cover most scenarios**

Reaction interface: Reduced Reaction Set

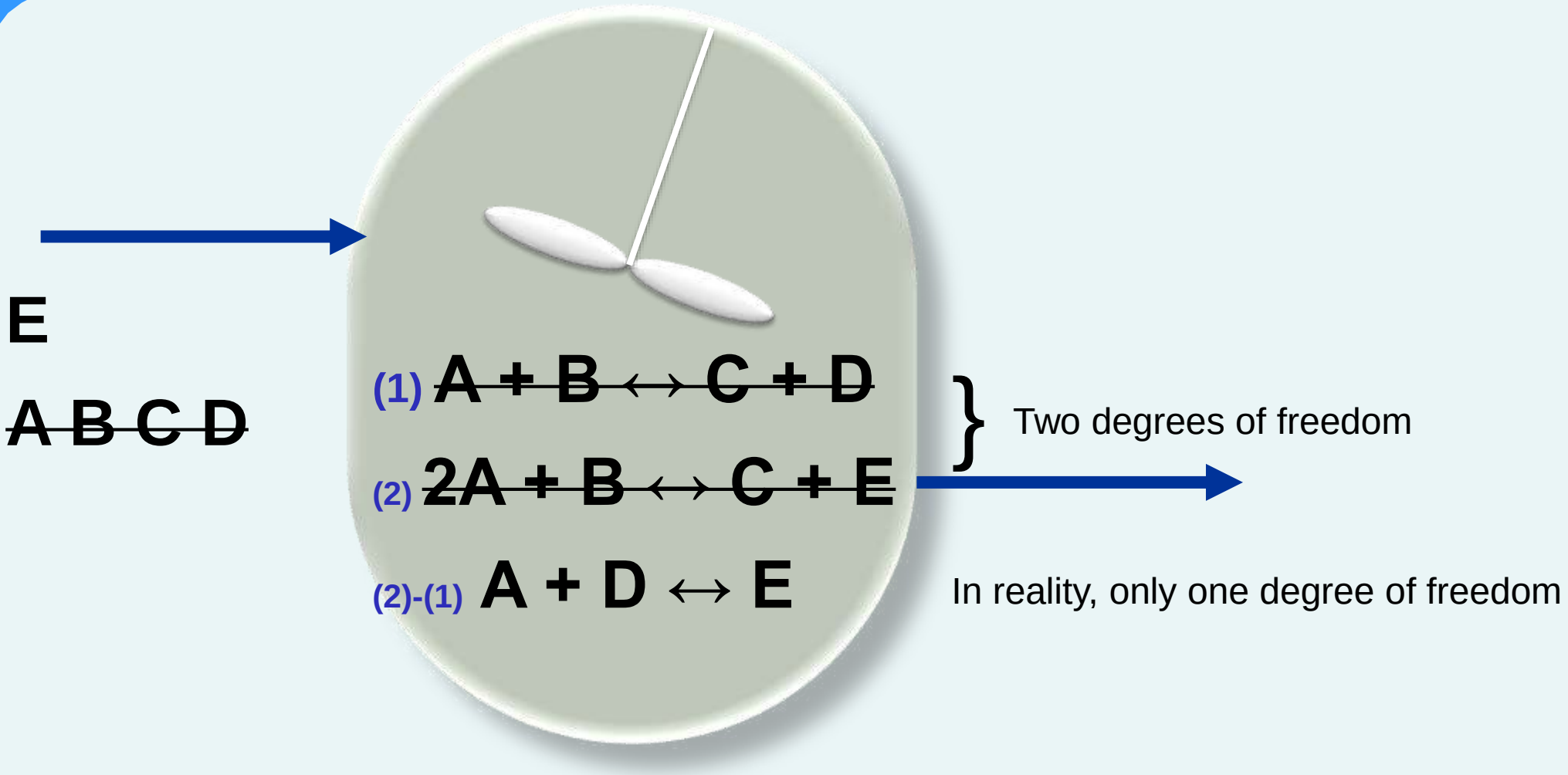


Reaction interface: Reduced Reaction Set



Reactions (1) and (2) may not take place by themselves, but cannot simply be discarded

Reaction interface: Reduced Reaction Set



System is singular when using original reactions

Reaction interface: Reduced Reaction Set

- If the set of reactions is not reduced, the full set of equations is degenerate
- Elimination and combination is a difficult problem, especially for many reactions
- Reactions cannot always be combined (depending on basis of equilibrium formulation)
- The responsibility for evaluating which reactions are possible, lies with Chemical Reaction Server, not with Reactor

Reaction interface: Reduced Reaction Set

- To allow transferring possible reactions: new concept "Reduced Reaction Set"
- Chemical Reaction Server provides Reduced Reaction Set based on defined compounds, defined phases and compounds absent from feed
- Reduced Reaction Set may contain new Reactions
- Lifetime of new Reactions coupled to Reduced Reaction Set lifetime
- Configuration of Material Template may require Reduced Reaction Set
- Reactor calculation may require Reduced Reaction Set

Concepts documented, methods introduced, Use Cases adapted done

Manager Common Interface

- **Thermo 1.1 uses Property Package Manager**
  - ***ICapePropertyPackageManager::GetPropertyPackageList***
  - ***ICapePropertyPackageManager::GetPropertyPackage***
- **Complicated Use Case: depersist property package:**
  - ***ICapePropertyPackageManager::GetPropertyPackage* is used and package creation is postponed until *Initialize***
- **Unfulfilled Use Case: create and configure property package:**
  - **All packages must therefore be created outside of CAPE-OPEN scope**

Manager Common Interface

- **Requirement: two more Property Package Manager functions**
  - ***CreateAndConfigureNewPackage***
  - ***CreatePackageForDepersistence***

Manager Common Interface

- Requirement: two more ~~Property Package~~ Manager functions
  - *CreateAndConfigureNew~~Package~~*
  - *Create~~Package~~ForDepersistence*
- Concept of a Manager is generic (not specific to thermo)
- Hence: Manager Common Interface: *ICapeManager*
- Cannot change thermo 1.1 (but 1.2? 2.0?)
- Opportunity to apply new interface to Reaction Package Manager
- ***Affects all lifetime related Use Cases in Reaction spec.***

Document change: to complete

- Business cases: insufficient resources
  - Omit
- For all Use Cases:
  - Will be revised pending Manager Common interface specification
  - Manager Common interface specification to be moved out from current Chemical Reactions interface specification

Summary and further actions

- **Immediate document changes**
  - **Mark Use Cases related to Manager Common interface specification as under construction**
  - **Remove interface design on Managers**

- **RFC for Reactions**
  - **Starting November 1, 2019**

- **Separate document for Manager Common interface specification**

Questions?

Thank you for your attention!

Go CAPE-OPEN!

CO LaN