

Thermo SIG Progress Report 2018

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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

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


Summary of activities 2017-2018




- **Custom Data interface specification**
 - **Issue: support missing for persistability of Custom Data**
 - **Solution: interface design modified**

- **Chemical Reactions interface specification v1.1**
 - **Issues: heat balance, incomplete Use Cases, missing business cases**
 - **Solution: new reaction property, improved Use Cases, -**

- **Errata Thermo 1.1**
 - **Diffusion coefficients: unclear definition**
 - **Solution: under discussion – round table session later this afternoon**

Goals set for 2018: comparison with expected

- **Custom Data interface specification**
 - Re-design made 
 - *RFC initiated*

- **Chemical Reactions interface specification**
 - **Formulation of business cases**
 - Some progress then stopped (lack of resources)
 - **Multiple Compound Slates (true and apparent)**
 - Textual requirements 
 - Use Cases 
 - Interface descriptions 

Goals set 2018: comparison with expected (cont.)

□ Chemical Reactions interface specification

■ Heat balance

- solution proposed
- examples to be worked out

■ Link between chapters done

■ Request For Comments (expected January, 2018)

• Delayed:

- lack of resources,
- unanticipated modifications in Custom Data (made mandatory in number of cases)

Custom Data

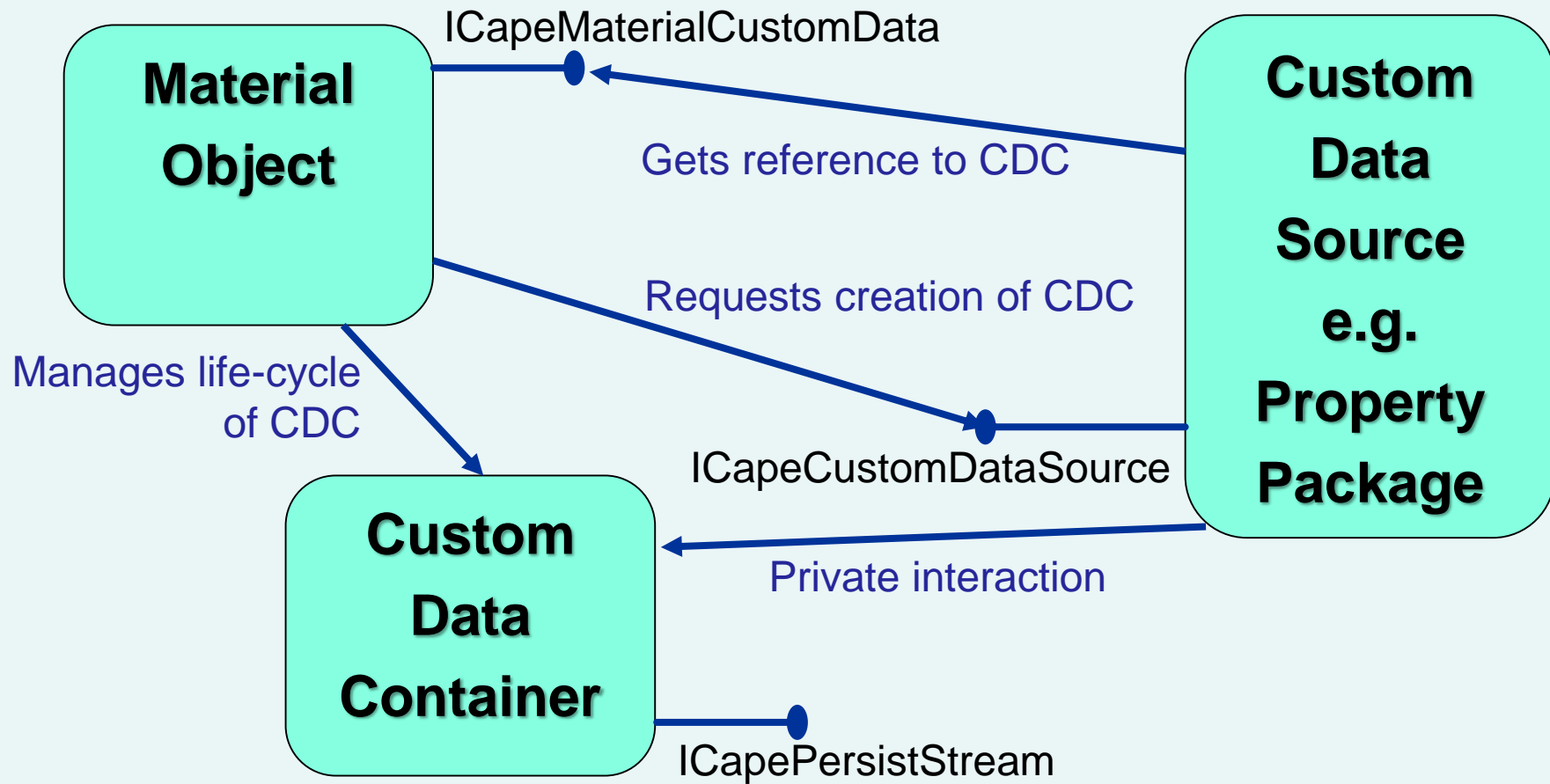
- **Custom data lie between PME and PMCs**
 - **Allows storage of PMC's specific data on Material Object**
 - **A means to improve performance of chemical equilibrium**

Custom Data redesign

- **Custom Data changed from CapeVariant to CapelInterface**
 - **Terminology redefined**
 - Custom Data Owner to Custom Data Source
 - Custom Data to Custom Data Container
 - **Allows persistability (inter-thread or inter-process)**
 - **Supports cloning**
 - **Threading issues resolved**



Custom Data model



Custom Data life cycle



□ Life cycle re-defined

- Custom Data Source provides method for creation of Custom Data Container
- Material Object handles life cycle of Custom Data Container
- One Custom Data Container per Custom Data Source per Material Object
- Custom Data Source identifies which Custom Data Container is requested
- Custom Data Container cannot be shared between multiple Material Objects
- Hint: Custom Data Source can implement sharing between Custom Data Containers in a copy-on-write manner

Custom Data RFC

□ **Interface specification document submitted for RFC**



▪ **CO-LaN membership asked to review**

□ **RFC deadline postponed to November 1, 2018**

▪ **Some comments already received: thanks**

▪ **CO-LaN members, please provide your comments**

□ **Analysis of comments underway**

Custom Data and reactions

- **Avoid repeating chemical equilibrium calculations**
 - **E.g. to access true composition in electrolyte systems**
 - **High impact on performance**

- **Mandatory support of Custom Data interface by PME**
 - **Chemical Phase Equilibrium applications**
 - **Multiple Compound States**

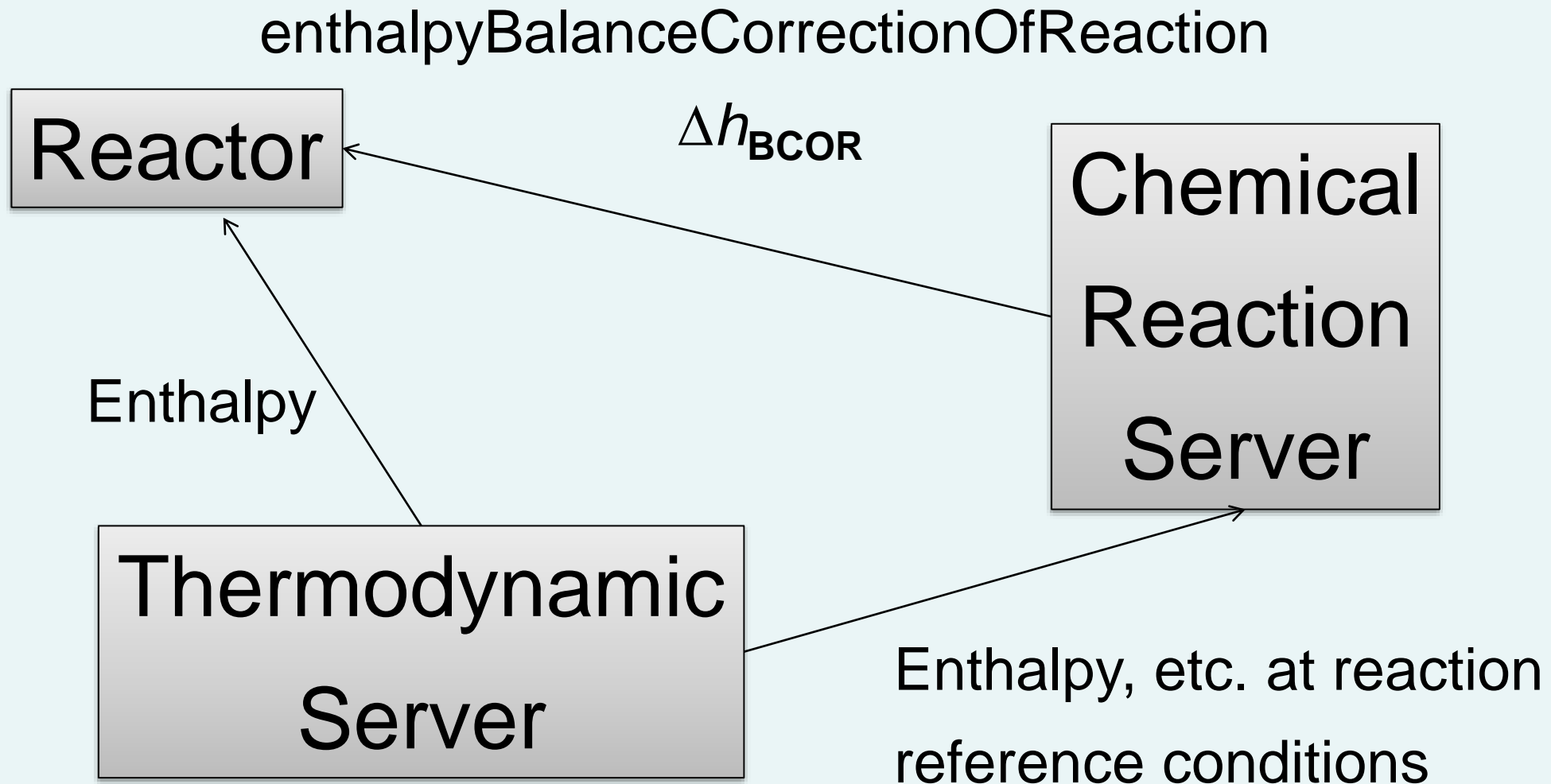
Chemical Reactions Interface Specification

- **Check reactions Use Case added**
 - **Validation of reactions made implicit part of validation of a Reactor**
 - **Examples**
 - **Validate that configured reactions are still available**
 - **Validate that the reaction domain fits with the reactor domain**
 - **Availability of stoichiometry or other reaction attributes**

Heat balance

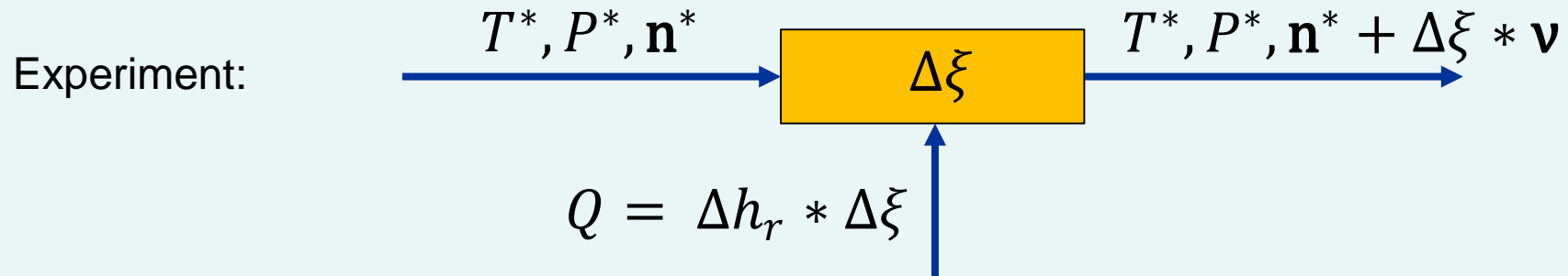
- Heat balance around Reactor
 - Accumulation = in – out + external duties +
[reaction contribution ?]
- The Chemical Reaction Server decides on how to compute the heat contribution of a reaction
- Chemical Reaction Server can access the Thermodynamic Server (via active Material Object)

How to set up a consistent heat balance?



Example from document

□ Heat of reaction as a single point value



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

$\Delta \xi \rightarrow 0$

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

known
to CRS

using Property Package

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

Heat balance

- Heat balance around Reactor
 - Accumulation = in – out + external duties +
[reaction contribution ?]
- The Chemical Reaction Server decides on how to compute the heat contribution of a reaction
- Chemical Reaction Server can access the Thermodynamic Server (via active Material Object)

Heat balance

□ Heat balance around Reactor

- Accumulation = in – out + external duties - $\sum \Delta \xi_i * \Delta h_{BCOR,i}$

□ The Chemical Reaction Server decides on how to compute the heat contribution of a reaction

□ Chemical Reaction Server can access the Thermodynamic Server (via active Material Object)

Document change: to complete

- **Business cases: insufficient resources**
 - **Separate document?**
 - **Omit?**
- **Document heat of reaction consistency issues**
 - **Completed in part through additional property Δh_{BCOR}**

Summary and further actions

- RFC initiated for Custom Data
 - Analysis of comments
- RFC for Reactions
 - Promised in January 2018 but not delivered
 - Unforeseen work
 - Lack of resources
 - Need to complete heat of reaction issues
 - As soon as done, RFC to be issued

Questions?

Thank you for your attention!



Go CAPE-OPEN!