

# Thermo SIG Progress Report 2016

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**Michel Pons, CO-LaN / France**

## 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

- ◆ Jasper van Baten
- ◆ Mark Stijnman
- ◆ Michel Pons
- ◆ Ryan Liu
- ◆ Jian Yong (Jim) Yang
- ◆ Richard Szczepanski
- ◆ AmsterCHEM (co-leader)
- ◆ Shell Global Solutions
- ◆ CO-LaN
- ◆ Honeywell
- ◆ Honeywell
- ◆ KBC ADVANCED TECHNOLOGIES (A Yokogawa company)
- ◆ Sergej Blagov
- ◆ Suphat Watanasiri
- ◆ Vicky Athanasiou
- ◆ BASF (co-leader)
- ◆ Aspentech
- ◆ Honeywell

# Thermo SIG Annual Report: Membership

- ◆ **Bjørn MARIBO-MOGENSEN (Hafnium Labs), formerly at DTU-CERE and Linde, joined last week the core team**
- ◆ **Thermo SIG is looking forward to work with Bjørn**
- ◆ **Experienced in electrolytes and CAPE-OPEN implementation**



# Activities 2015-2016

## ◆ Mark Stijnman joined the core SIG activities

- Reviewed extensively current document

## ◆ Efforts concentrated on the Chemical Reactions interface specification v1.1

- Main ideas first presented on CO-LaN Annual Meeting, 2012, Lyon, France

## ◆ Ongoing work in a small group

- Jasper van Baten, Mark Stijnman, Michel Pons, Sergej Blagov
- 2 hours weekly remote desktop sessions

## ◆ *Still* not finished

- ◆ **Where we stand (mid-April 2016):**
  - **Requirements finalized and classified per package**
  - **Use Cases finalized (29)**
- ◆ **Not finished**
  - **Interface method documentation**
  - **Interface formalization (IDL)**

- ◆ **We requested reviews from other parties for check of completeness and consistency**
  - **Extensive review from Mark Stijnman received**
  - **Basic questions on the document were raised**
    - **Need for clarifications on business cases**
    - **Less recommendations, stricter rules (refer to CO 2015)**
    - **Overly complicated hierarchy of reactions (introduced in 2015)**
    - **Global document structure**
      - **CAPE-OPEN template improper?**
      - **Splitting document in different scope sections**

# Immediate goals (1)

- ◆ **Formulation of business cases**
- ◆ **Restructuration of document**
  - **Document treats three concepts**
    - A Reaction Server that exposes reactions
    - A Chemical Phase Equilibrium Server
    - Multiple Compound Slates (true and apparent)
  - **Initial structure follows CAPE-OPEN template**
    - Textual requirements, Use Cases, Interface descriptions
  - **Proposed structure: separate by concepts**
    - CAPE-OPEN template applied per concept



# Immediate goals (2)

- ◆ Means to achieve these goals
  - Formulate theoretical background with consistent terms and symbols for use in business cases and throughout document
- ◆ Purpose is not to write a textbook but
  - Motivate interface design
  - Demonstrate how interface design fits with common reaction engineering modeling approaches

# Business cases

- ◆ Explain expectations of Reaction Package standard:
  - Enumerating example fields of applications:
    - e.g. electrolytes, reuse of reaction definitions between reactors,...
  - Product management issues:
    - e.g. minimum functionality, IPR, package configuration,...
- ◆ Justify interface design
  - Reactive Equilibrium distinct from Phase Equilibrium
- ◆ Introduce and help navigate through major concepts of the interface:
  - e.g. Reaction server, Chemical Reaction Equilibrium, Multiple compound slates

# Currently out of scope

## ◆ Polymerization

- No standardized approach for population balances

## ◆ Field-induced reactions

- External driving force
- Production and consumption on non-compounds
- Examples: electric current, radiation (X-ray, light, ...)

## ◆ Petrochemical reactions

- Externally defined reactions are unable to affect petrochemical properties (e.g. sulfur content)

# Summary

- ◆ **Main building blocks are available**
  - **Textual requirements, Use Cases**
  - **Is it time to prototype current design?**
- ◆ **Re-arrangement of document envisioned**
  - **Per main concept**
- ◆ **Hierarchy of reactions challenged: change in design?**
- ◆ **More feedback is welcome from CO-LaN membership**
  - **Especially from parties interested in implementing**
  - **Current documents are available to all Members**

# Questions?

Thank you for your attention!



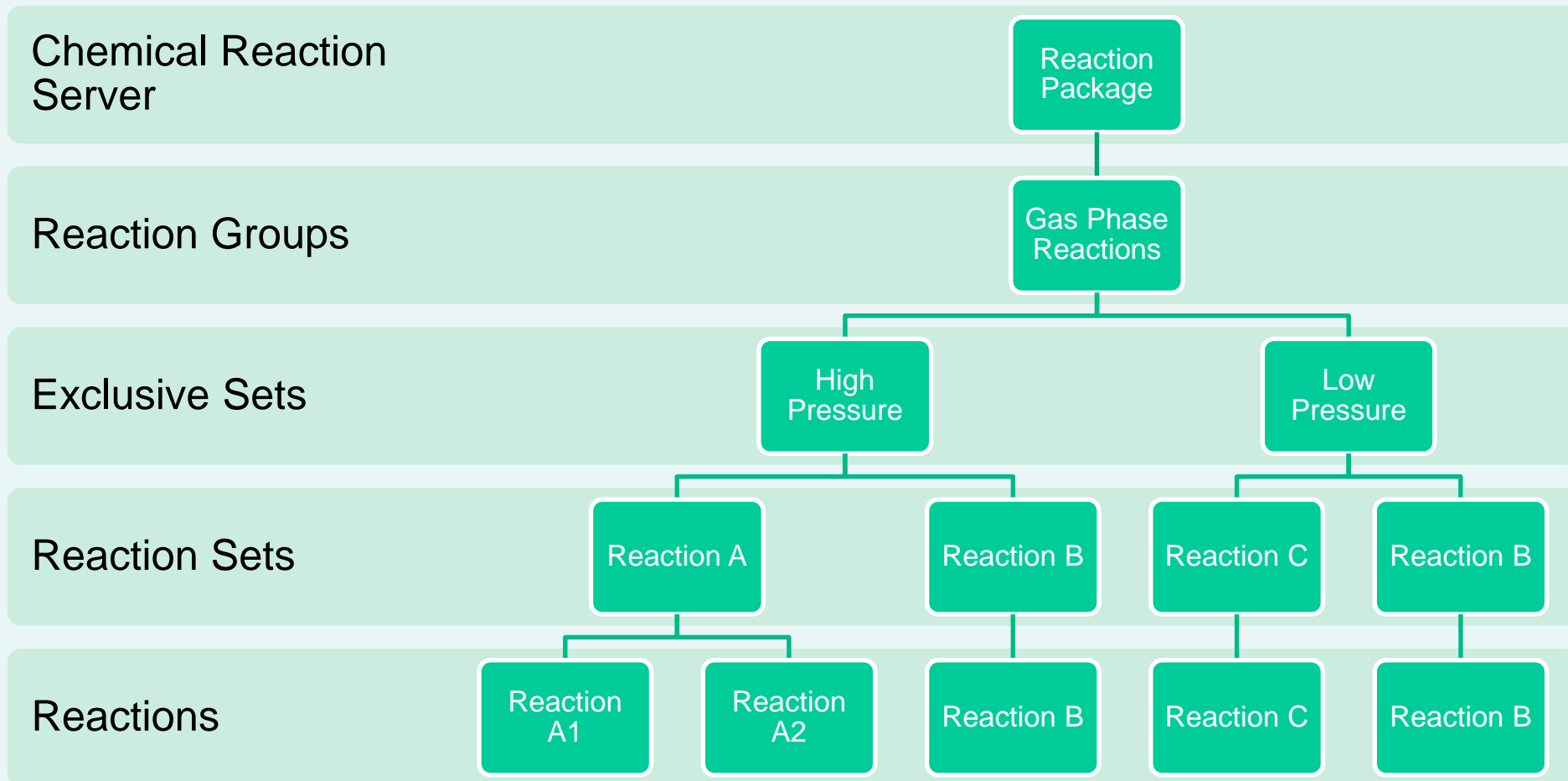
Go CAPE-OPEN!

# Main concepts: Chemical Reaction Server

## ◆ New:

- **Reorganization of reactions into a hierarchy**
  - **Reaction groups**
    - Arbitrary grouping of reactions related to each other
  - **Exclusive sets**
    - Groups of mutually exclusive reactions at alternative conditions
  - **Reaction sets**
    - Groups of reactions that must be evaluated together
  
- **Advantages of the generic approach proposed**
  - Ease of analysis by the PMCs using CRS
  - Complex reaction systems are easily defined

# Internal representation



# Example of GUI representation

Select reactions:

- High Pressure Reactions
  - Reaction A
    - Reaction A1
    - Reaction A2
  - Reaction B
- Low Pressure Reactions

Reaction Package

Gas Phase Reactions

High Pressure

Low Pressure

Reaction Sets

Reaction A

Reaction B

Reaction C

Reaction B

Reactions

Reaction A1

Reaction A2

Reaction B

Reaction C

Reaction B



# Main concepts: Multiple compound slates

