Thermo SIG Progress Report 2015

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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

- As of October 2015
  - Andrew Lintern, HTRI
  - **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

Thermo SIG Annual Report: Activities 2014-2015

- **Efforts concentrated on finalizing 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, Michel Pons, Sergej Blagov
  - 2 hours weekly remote desktop sessions
- ***Still* not finished**

Chemical Reactions Interface v1.1: Motivation

- **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
- **CO-LaN Annual Meeting, 2012, Lyon, France:**
  - First draft presented
  - Major drawbacks recognized:
    - *Formulation only based on the true species*
    - *Not well suited for oligomers, electrolytes*, etc.
    - *No reactive phase equilibrium calculator defined*

Chemical Reactions Interface v1.1: Key Features

- **Generality**
  - Phases for reactants and products on a per-component basis
  - Reaction domains: single phase, interfacial, homo-/hetero-geneous, etc.
- **Compactness**
  - Only 4 reaction properties supported
    - Reaction Rate / Compound Reaction Rate
    - Chemical Equilibrium Deviation
    - Chemical Equilibrium Deviation tolerance
    - Enthalpy of Reaction
- **Flexibility**
  - Reaction hierarchy
  - Multiple Compound Slates (for different sets of apparent compounds)
  - Material Object Delegates in addition to Material Object

Chemical Reactions Interface v1.1: Main concepts

- Chemical Reaction Server
- Reactive Phase Equilibrium
- Compound Slate
- Custom Data storage on Material Object

Main concepts: Chemical Reaction Server

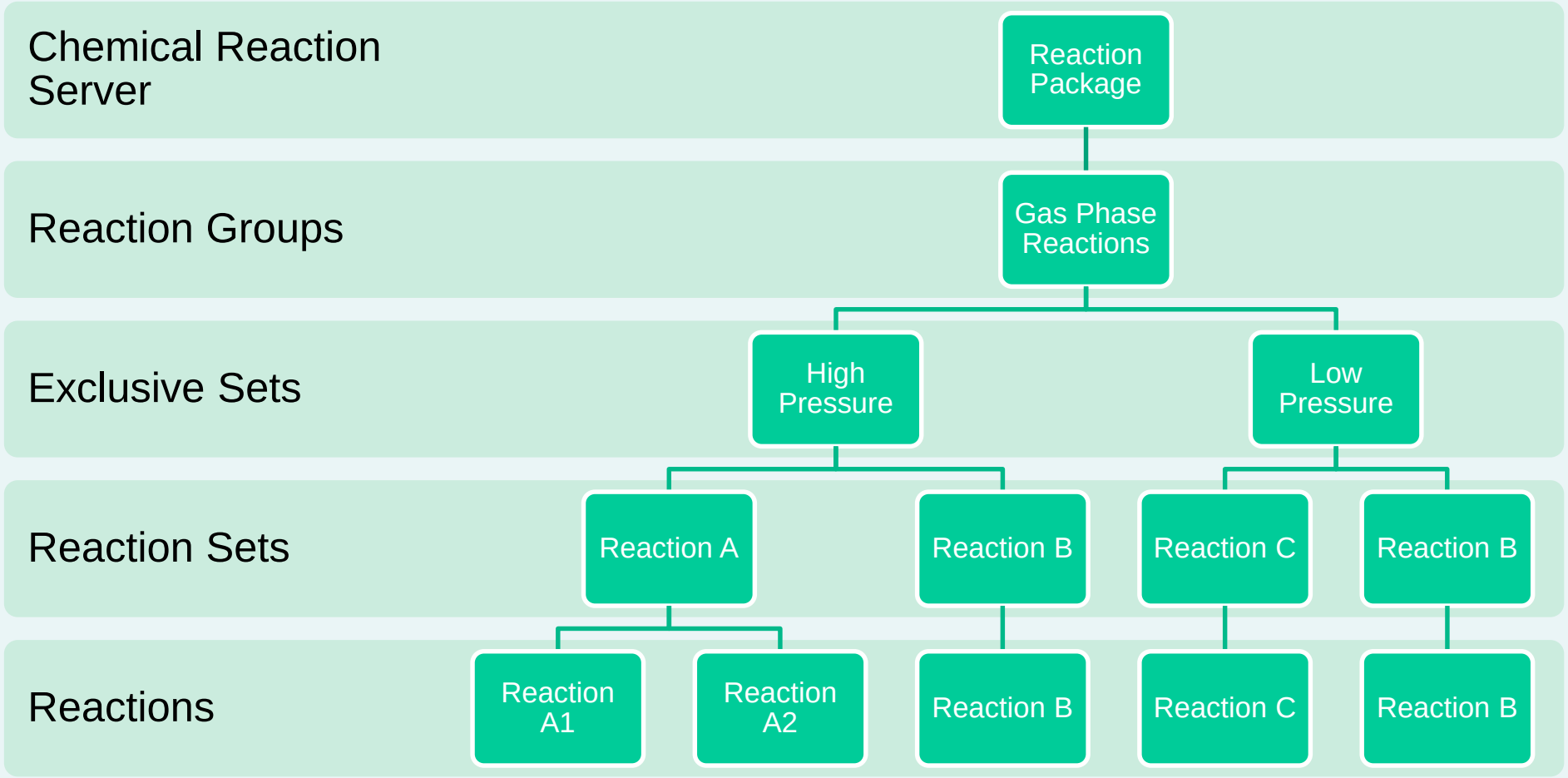
- Either a Property Package or a Reaction Package
  - Concept already presented in 2013

- Levels of configuration
  - Chemical Reaction Server private configuration
    - Outside of PME or via ICapeUtilities::Edit if supported
  - Association with Material Template
    - Matching of compounds and phases
    - Selection of reactions supported by the Material Object
  - Association with Unit Operation
    - Via Material Object representing feed or product stream
    - Possible selection of reaction subset by Unit Operation
    - Selection must be consistent with reaction hierarchy

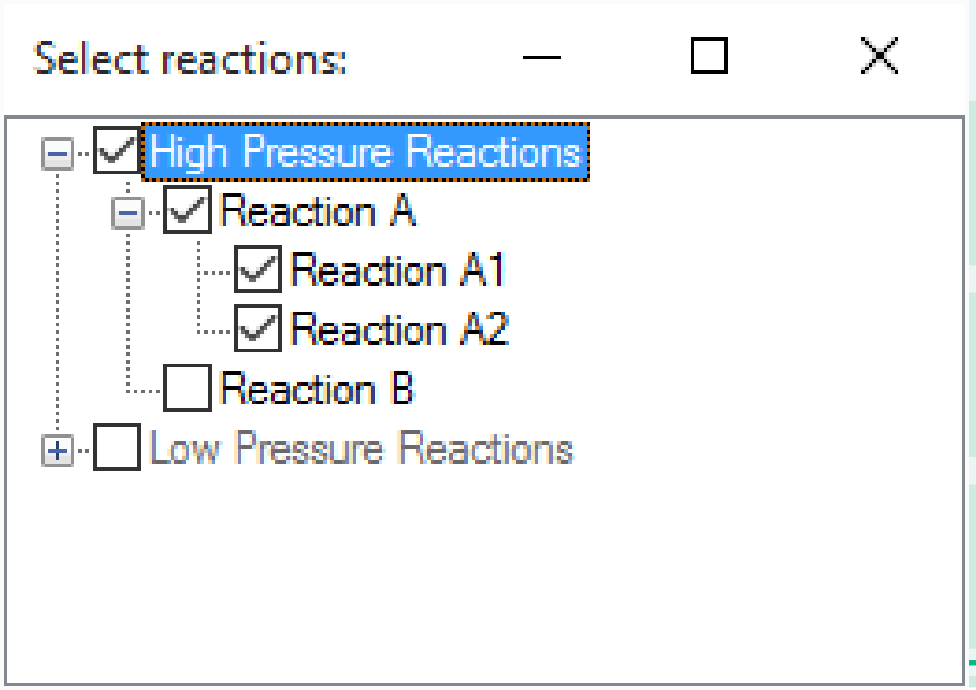
Main concepts: Chemical Reaction Server

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

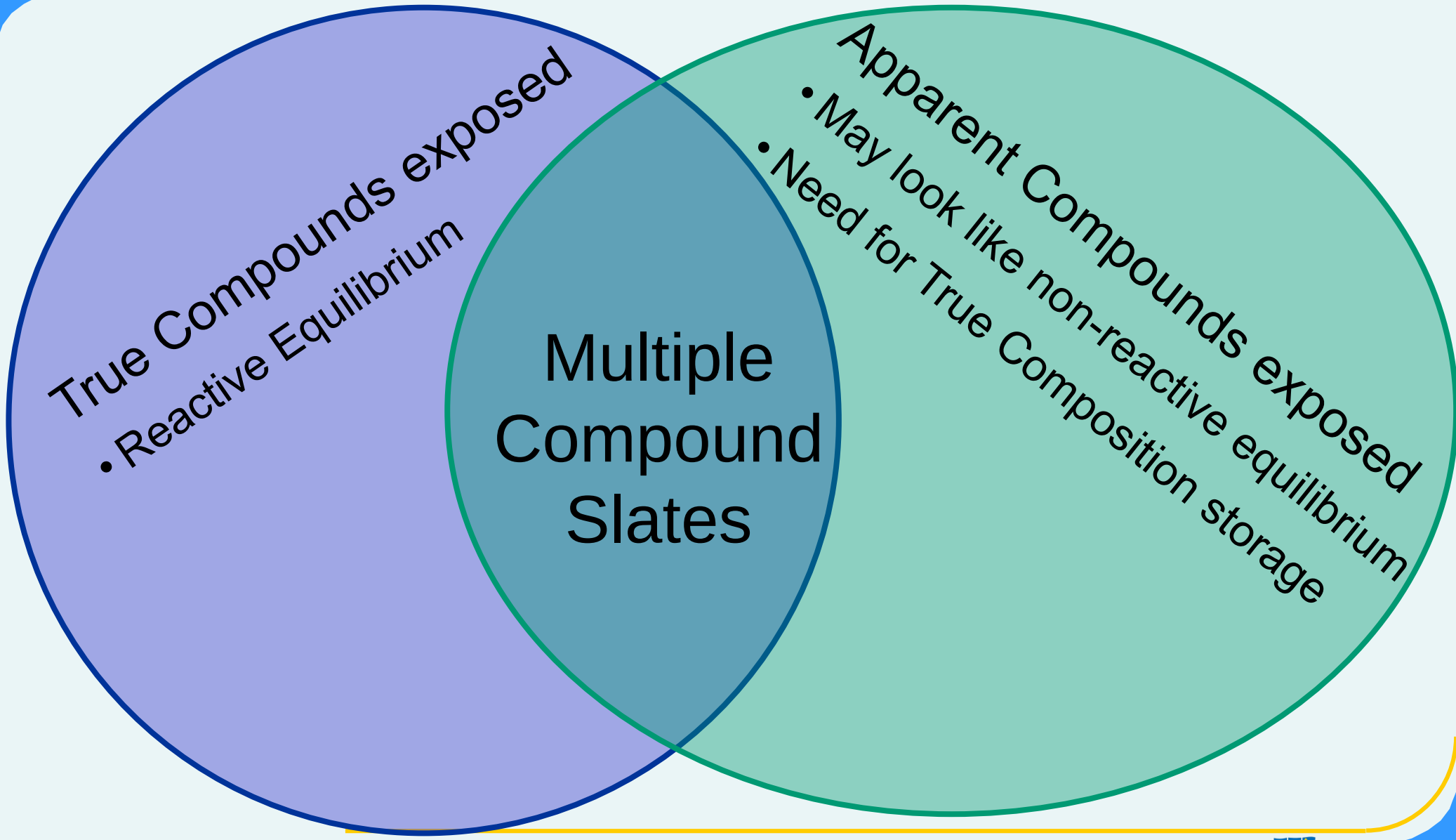
Internal representation



Example of GUI representation



Equilibrium reactive systems

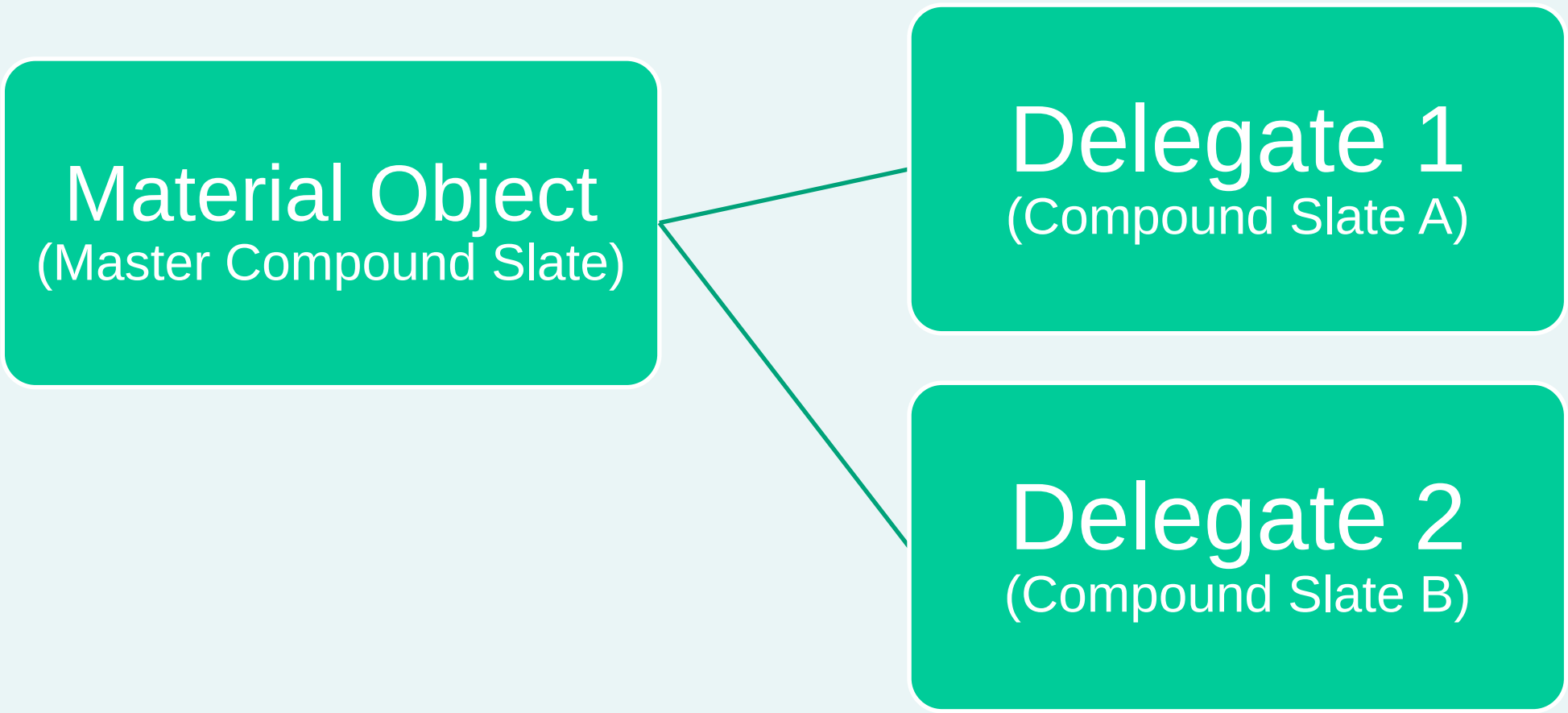


Main concepts: Reactive Phase Equilibrium

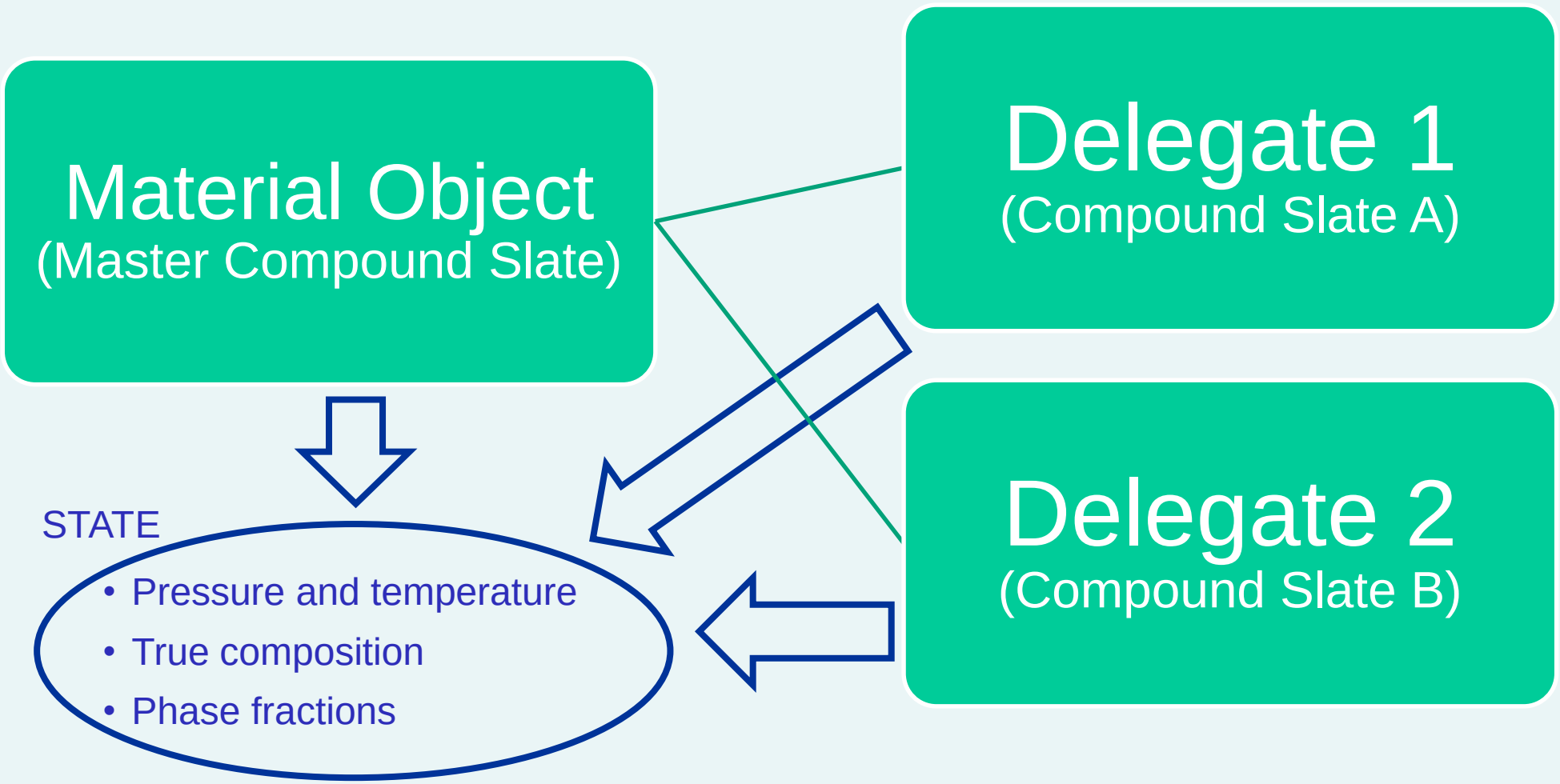
- Reactive Phase Equilibrium changes overall composition

- Unit Operation must be aware of this change
  - Molecular weight changes
  - ICapeThermoReactiveEquilibriumRoutine
    - As discussed last year

Main concepts: Multiple compound slates



Main concepts: Multiple compound slates



True composition internal to Property Package

- Typical sequence of events
  - True composition calculated as part of phase equilibrium
  - Phase equilibrium often followed by property calculation
  - Property calculation requires true composition

True composition internal to Property Package

- Recalculate true composition
  - CPU intensive
- True composition cached on Property Package
  - Inconvenient
    - no knowledge of life-span of each Material Object
    - no knowledge on number of Material Objects
- Storage of true composition on Material Object
  - New interface: Custom Data

Main concepts: Custom Data on Material Object

- Generic or specific interface design
  - Format not known to Material Object: specific to PMC
  - Other usages: for example EOS solutions

- Rules
  - PMC must store data along with applicable conditions
  - PME must remove data when thermo configuration changes
  - PME not required to persist data
    - PMC must be able to recalculate data
  - Guidelines for multithreading and sharing data between Material Objects

Points progressed

- **Formalized all requirements**
  - **Ensured consistency with the design chosen**
    - **Revised most of the requirements**
  - **Split into three sections**
    - **Chemical Reaction Server**
    - **Reactive phase equilibrium**
    - **Multiple compound slates**
- **Working on Use Cases**
  - **Remains finalizing Use Cases and interfaces**
- **Separate document on Custom Data storage**
  - **To be distributed along with Chemical Reaction**

Questions?

Thank you for your attention!