Thermo SIG Progress Report 2022

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Thermo SIG Annual Report: Charter

Scope:

- Thermodynamics and Physical Properties interface specification v1.0 (deprecated)
- Thermodynamics and Physical Properties interface specification v1.1 (active)
- Chemical Reactions interface specification v1.1 (under development)
- Custom Data interface specification v1.1 (active)
- Compound Server interface specification (draft only)

and related documents, files, tools, software, and procedures.

Thermo SIG Annual Report: Charter

Key Responsibilities:

- Maintain and manage active interface specifications (revisions to improve design, performance/speed and robustness based on user input)
  - Provide errata and clarifications and integrate in current specification
- Assess and prioritize on expansions of thermodynamic interface specifications
- Help member organizations to develop implementations of thermodynamic interfaces
  - Provide advice on migrating from deprecated to active interface versions
  - Provide advice on new implementations
  - Analyze interoperability issues between PME and PMCs
- Define compliancy tests for thermodynamic interface specifications

Thermo SIG Annual Report: Membership

- Sergej Blagov
- Jasper van Baten
- Klaus Möller
- Michel Pons
- Bjørn Maribo-Mogensen
- Mark Stijnman
- Richard Szczepanski
- ?
- ?

- BASF (co-leader)
- AmsterCHEM (co-leader)
- University of Cape Town
- CO-LaN
- Hafnium Labs
- Shell Global Solutions
- KBC Advanced Technologies Ltd
- AspenTech
- Honeywell Process Solutions

Summary of activities 2021-2022

- Chemical Reaction Specification document
  - Revision according to comments received
    - Extensive review from Linde Engineering. Much appreciated.
      - resulted mostly in clarifications brought in the document,
      - few modifications made to interface design.
- Specification document for a Manager Common Interface
  - Requirements and interface design developed
  - Documentation status: 15 requirements, 8 Use Cases
  - In the process of finalizing draft

Motivations behind Manager Common Interface

- A generic interface for Property Package Manager (PPM), Reaction Package Manager (RPM), (Unit Operation Manager?)
- Deals with shortcomings in *ICapePropertyPackageManager*
- Really a Common Interface:
  - Methods & Tools SIG responsibility
  - Avoids duplication of similar functionality for different PMC types
- Finds first application in Reaction Package Manager
- Needs to be published in order for Chemical Reactions specification to be completed

A Manager defines Templates

- A Template is not a CAPE-OPEN object
- Templates are reusable
- *Contains a configuration of a PMC to be created by the Manager*
- Only Template name is visible through CAPE-OPEN
- Upon creation of PMC, Template is used for initial configuration
- Template and configuration of PMC created from Template are decoupled; changing PMC configuration does not affect the Template

Limitations of current published interfaces

- ICapeThermoPropertyPackageManager:
  - Only supports creation of Property Package (PP) from Template name (Package name)
  - Creation from persistence cumbersome:
    - Issues on all objects involved: PME, PPM and PP
      - When asking for creation of PP, PME cannot state its intent to de-persist PP after creation, but PME must specify a package name.
      - Package name specified for creation has no meaning for the PPM in case of subsequent de-persistence by PME.
      - Package name error handling is therefore postponed to a later call to ICapeUtilities::Initialize on PP.
  - Creation of PP from scratch not part of ICapeThermoPropertyPackageManager interface
    - No standard way to create a new PP directly from within PME

Examples of Templates

Template contains a configuration for a PMC:

- **Property Package Template**
  - **Selection of compounds, phases, models and associated data**
  - **Specialized PPMs may have a useful default for which no Template is needed (e.g., specialized air separation PPM)**
- **Chemical Reaction Package Template**
  - **Selection of compounds, reaction stoichiometries, …**
- **Unit Operation Manager**
  - **Does not yet exist. Your feedback?**
  - **Example: Distillation Column Manager**
    - **Template: Selection of internals, reboiler, condenser, draw-offs, …**
    - **Default Template: perhaps a simple distillation column**

Manager Common Interface

- Design objective:
  - Intent of PMC creation to be stated by PME
- Design: Manager supports 3 ways of PMC creation:
  - From Template
    - Note: managing of Templates (creation, deletion, renaming, etc…) is internal to the Manager (ICapeUtilities::Edit and/or external app)
  - From persistence
    - Requirement: a PMC created via a Manager implements persistence
  - From scratch (optional)
    - Avoids creation of Template that has no further use as a Template
- All Manager types have stand-alone equivalents:
  - Example: PPM vs stand-alone PP

Create from Template

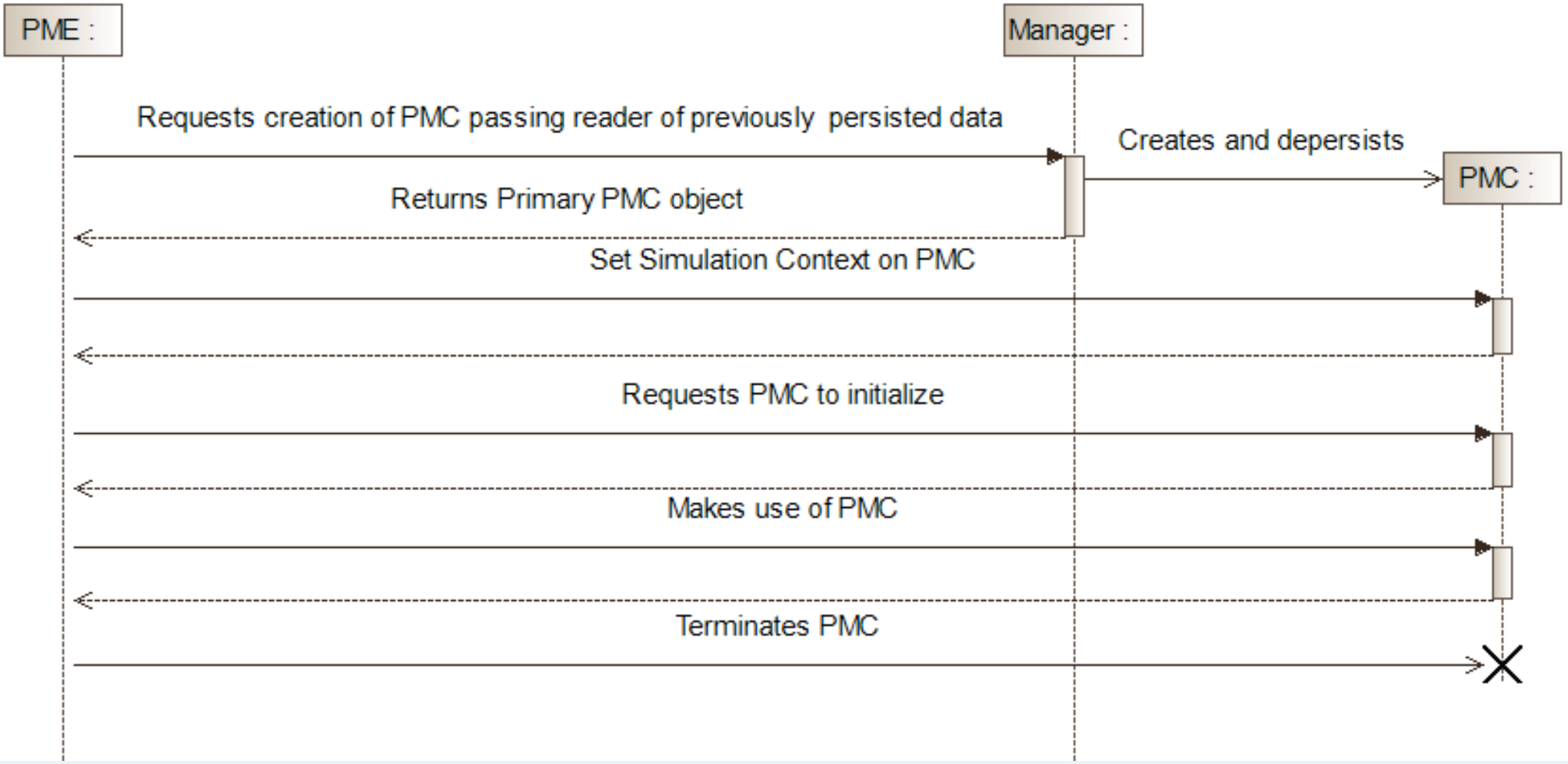
- Pick Template from list, and create PMC
- Similar procedures as in *ICapeThermoPropertyPackageManager*
  - GetTemplateList versus GetPropertyPackageList
  - CreateFromTemplate versus GetPropertyPackage

Create from persistence

- PMCs created by Manager must implement persistence
  - To stimulate portability
  - Minimal implementation (not recommended):
    - Just persist Template name (not portable)
  - PME no longer needs to persist Template name

- De-persistence is a single operation requested on Manager
  - *ICapeManager::CreateFromPersistence*
  - Returns the de-persisted PMC to PME

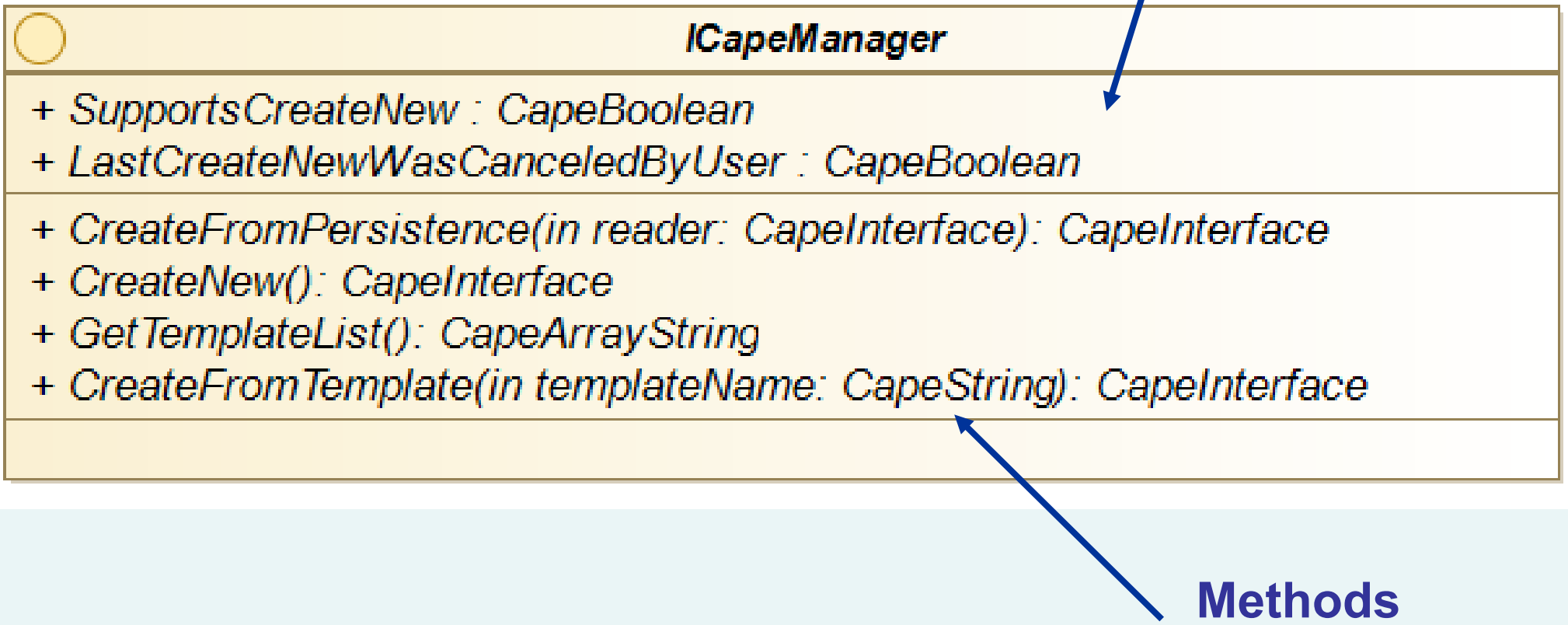
Create from persistence



Create from scratch (Optional)

- Purpose: one-off PMC for use in current application without need for a Template
- Manager is allowed (and expected) to show a modal GUI for configuring new PMC. PME should be prepared for this.
- Methods:
  - *SupportsCreateNew*: allows PME to arrange its GUI
  - *CreateNew*: returns newly created PMC
    - Manager may allow initial configuration of PMC through GUI
    - User may cancel creation: raise a CAPE-OPEN error
  - *LastCreateNewWasCanceledByUser*: allows PME to determine whether to show creation error in case of user cancel

Manager interface



Roadmap

- Manager interface: part of CAPE-OPEN 1.1
  - Consistent and to be used with Chemical Reactions interface specification 1.1
- Property Package Manager interface not deprecated from CAPE-OPEN 1.1
- When to deprecate PPM interface?
  - Not CAPE-OPEN version 1.2
  - CAPE-OPEN 2.0?
- Additional Manager types may appear in CAPE-OPEN 1.2
  - E.g. Unit Operation Manager

Outlook 2022-2023

- Work outlined for this year:
  - Support:
    - Certification support: define the tests (Laborious!)
    - Maintain and manage existing interface specifications
  - Manager Common Interface proposal
    - Hand over to Methods & Tools (M&T) SIG for finalizing
    - Suggest Unit Manager to Unit SIG?
  - Publish Chemical Reactions interface specification
    - Act on RFC, publish IDL, disseminate

Questions?

Thank you for your attention!

Go CAPE-OPEN!

CO LaN