Use of CAPE-OPEN standards
A solution to diffuse Thermodynamic Property Packages during the development cycle of a process

Philippe Arpentinier l Centre de Recherche Claude-Delorme Paris Saclay l Scientific Direction

CAPE-OPEN 2012 European Annual Conference
September 19-20, 2012 – Lyon, France

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■ **Definitions and Context (PME, PMC, TPP)**

■ **Tests of different TPPs in different PMEs**

■ **Conclusions and perspectives**

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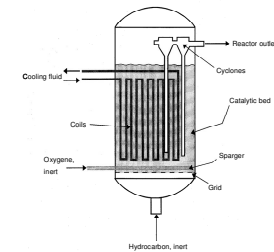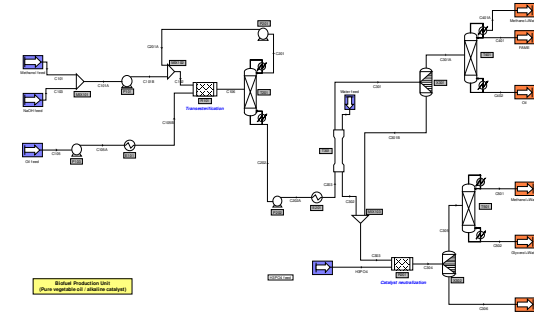- **Conclusions and perspectives**

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Definitions

- **PME: Process Modeling Environment**
  - **General environments intended to facilitate creation of process models, either starting from basic principles, or starting from libraries of existing models (PMCs), or both**
  - **Aspen-Hysys, Prosim Plus, Aspen-Plus, Pro II, Belsim-Vali, Unisim Design**
- **PMC: Process Modeling Component**
  - **Model of unit operation**
    - **Chemical reactor**
    - **Heat exchanger**
    - **Distillation column**
    - **...**
  - **Numerical methods**
  - **Thermodynamic Property Packages**

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Definitions

- **TPP : Thermodynamic Property Package**

    - **List of pure compounds**

    - **Properties of pure compounds (coming from a database)**

    - **Equation of state dedicated to the vapor phase**

    - **Equation of state ($\varphi - \varphi$ approach) or Activity coefficients models dedicated to the liquid phase ($\gamma - \varphi$ approach)**

    - **Mixing rules**

    - **Matrix of binary interaction parameters**

    - **Model or correlation for the calculation of liquid molar volume and fugacity of pure liquid in standard state**

    - **State reference of enthalpy and entropy calculation**

    - **Algorithm of resolution of phase equilibrium equations**

    - **Calculation methods of transport properties (thermal conductivity, viscosity, surface tension)**

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Air Liquide context

■ **Globalization of R&D and Engineering Departments (Europe, USA, Asia)**

- **Multiplicity of PMEs**
- **Cohabitation of different PMEs (R&D, Engineering Departments): Aspen-Hysys, Aspen Plus, Belsim-Vali, Prosim Plus, Unisim Design**

■ **Adoption of a thermodynamic standard usable at each step of process development**

- **Server of thermodynamic models and associated resolution algorithms: Simulis Thermodynamics**

  Software component for computing thermophysical properties and phase equilibria on pure components or mixtures in MS-Excel (Add-In functions), Matlab® or any CAPE-OPEN PME in the form of TPP able to be plugged

■ **Encapsulation in Simulis Thermodynamics (following CAPE-OPEN standard Thermo 1.0 and 1.1) of our in-house thermodynamic equation of state dedicated to air ternary system**

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Air Liquide context

- **Use of native thermodynamic models of Simulis to create CAPE-OPEN compliant TPPs**
  - Fitting of PR equation of state (coming from Simulis) on experimental measurements and diffusion as CAPE-OPEN TPP (separation/purification of carbon monoxide)
  - Extension of the validity range of Sour Water electrolytic model (addition of nitric acid dissociation) and use for CO_2 capture process simulation

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Tests of different TPPs CO compliant in PMEs

- **Test of proprietary TPP "Bender" in different PMEs**
    - **Operating system: Windows XP**
    - **Created from Simulis 1.4.1.0 (Thermo 1.0 and 1.1 compliant)**
    - **Simulation of a distillation column**

  - **Prosim Plus 3.2.0.1 → OK**

  - **Aspen Plus 7.2 → OK**

  - **Aspen-Hysys 7.2**
      - **TPP "Bender" returns an empty list of constant properties → generation of error messages**
      - **Help of CO-LaN to fix the bug**
          - **No question of providing our proprietary TPP to AspenTech**
          - **The problem was documented by CO-LaN by using a modified version of the thermodynamic examples carried out by AmsterCHEM for CO-LaN**
          - **In this way, AspenTech could have the source code of a software component highlighting in Aspen-Hysys a similar behavior**
      - **Problem normally fixed in release 8.0 (beta version)**

  - **Unisim Design R400 → OK**

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Tests of different TPPs CO compliant in PMEs

- **Test of "Sour Water" TPP in Belsim-Vali 4.7.0.3 (Thermo 1.0)**

  - **Operating system: Windows XP**
  - **Created from Simulis 1.4.1.0 (Thermo 1.0 and 1.1 compliant)**
  - **Simulation of CO_2 capture from oxy-fuel combustion flue gases (quench, SOx absorption, compression and inter-cooling steps)**

  - **"Sour water": electrolytic model**

    - **Heterogeneous approach $\gamma - \varphi$**
    - **Apparent species – Actual species (ions)**

      $[CO_2]app = [CO_2 (aq)] + [CO_3^{2-}] + [HCO^{3-}] + [H_2CO_3]$
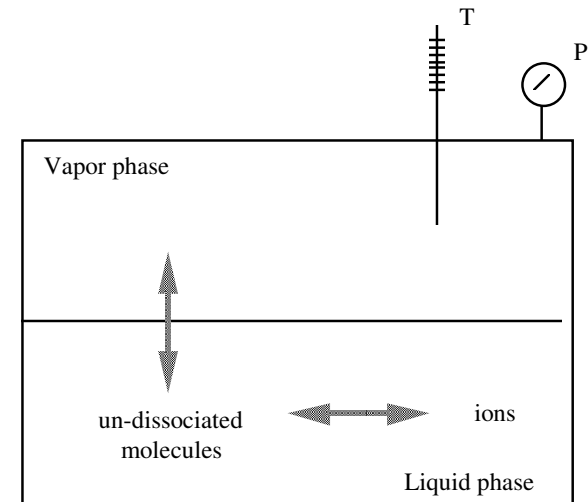
  - **Encouraging results**

    - **+++ : it works, Thermo 1.0 standard allows to treat electrolytic model**
    - **-- : increase of CPU time**
    - **Adaptation of Thermo standard to electrolytic models (SIG Thermo) ?**

Tests of different TPPs CO compliant in PMEs

■ **Another feedback**

    ▫ **Analytical derivatives compared to numerical derivatives**

        ■ **CPU time**

        ■ **Robustness**

    ▫ **Even if the analytical derivatives are available in the TPP, it happens that the PME still uses numerical derivatives !**

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Conclusions et perspectives

■ **Great interest for Air Liquide regarding the implementation of CAPE-OPEN interfaces in PMEs**

- **Aspen-Hysys**
- **Aspen Plus**
- **Prosim Plus**
- **Belsim-Vali**
- **Unisim Design**

■ **Appropriation of the concept of CAPE-OPEN TPPs dedicated to given applications and able to be plugged "everywhere"**

- **Interoperability of packages: PMEs, Excel, Matlab**
- **Consistency of results throughout different applications**
- **Perpetuation of in-house knowledge: database of packages**
  - **Detailed description and validity range**
  - **References of experimental values (literature, proprietary)**
- **Improvement of accessible information quality for a relevant later re-use**

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Conclusions et perspectives

- **Diffusion from R&D to other AL departments of CAPE-OPEN compliant TPPs generated with Simulis**
  - Improvement of the communication between Air Liquide departments
  - Improvement of the communication between Air Liquide R&D and academic partners

- **Support of PME suppliers to fix bugs linked to the implementation of the standards**
  - With the help of CO-LaN !

- **Adaptation of the Thermo standard to treat more efficiently models dedicated to electrolytic solutions ?**

- **To develop the same approach for unit operation models**
  - To make proprietary chemical reactor models developed between 1990 and 2005 (in only one PME) CAPE-OPEN compliant

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