Interoperability between Modelling Tools (MoT) and Process Simulators (ProSim) through CAPE-OPEN Standards

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Outline

• Objective
• Computer Aided Process Engineering Tools
  – MoT
  – ProSim & CO Interface (SIMULIS & Wrapper)
• Integration of MoT-ProSim
• Case Study
  – Thermo-Interface (External-Model:PC-SAFT)
  – Unit-Interface (Model:Short-Path Evaporator)
• Conclusions
Highlight aspects of interoperability of software tools through the application of Computer-Aided Modelling tools (for generation and use of Modelling Objects) in CAPE-OPEN compliant process simulators

*more specifically, uses of CO- interfaces for thermo-models and unit operations are demonstrated*
1. MoT

2. ProSim
   - Simulis thermodynamics
   - CO-wrapper
   - ProSimPlus
Computer Aided Process Engineering Tools

1. MoT

MoT Interface

- Model Definition
- View Original Model
- View Translated Model
- Input Model
- Model Grad
- Model Module

Model Variable Analysis
- Clearly Variables
- Variable Encoding
- Equation Ordering
- Set Variable Scaling
- Advanced Options
- Design Variables
- Constraint Variables
- Obj Value and Ranging
- Define Relationships
- Equation Traceback

Testbed Environment
- Define Compounds
- Define Streams Composition
- Data Sets
- Experimental Measurement

Model Information Retrieved
Model Testbed ver. 0.7

MoT Internal Diagnostics:
- $\theta = \text{Theta}^\circ_{\text{m}} + \text{Theta}^\circ_{\text{k}}$
- $\mu = \text{Mu}_{\text{m}} + \text{Mu}_{\text{k}}$
- $k = \text{K}_{\text{m}} + \text{K}_{\text{k}}$

Boundary condition at $y = 0$

$G_0 = 0$

Internal discretisation points:
- $G_1 = (\text{Theta}_1 - \text{Theta}_2 + \text{Theta}_3)/3$
- $G_2 = (\text{Theta}_2 - \text{Theta}_3 + \text{Theta}_4)/3$
- $\vdots$

Boundary condition at $y = 1$

$G = \text{Theta}_{10} - \text{Theta}_9 + \text{Theta}_10$

Flow rate in the liquid and vapour phase (mol/s):
- $\text{Flow}_{\text{L}} = \text{Flow}_{\text{V}}$
- $\text{Flow}_{\text{V}} = 2 \cdot \text{Flow}_{\text{L}}$
- $\text{Flow}_{\text{L}} = \text{Flow}_{\text{V}}$

$T_{\text{mix}} = T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7 + T_8 + T_9 + T_{10}/10$

$Q = 0$
1. MoT

![Image of MoT software interface]

- MoT
- ProSim
- ProSim Plus

Model Information Retrieved
Model Tested ver. 0.7

Model Definition

- Model Definition
- View Original Model
- View Translated Model

Input Model

- Input Model
- Create Model

Modify Model

- Modify Model
- Model/Variable Analysis

- Advanced Options

- Design Variables
- Constraint Variables
- Ouput variables
- Equation Ordering

- Solve Variable Value

- Data Sets

- Experimental Measurements
1. MoT
1. MoT
1. MoT
Computer Aided Process Engineering Tools

1. MoT

MoT

ProSim

ProSim
1. MoT

**ProSim**

Computer Aided Process Engineering Tools

![ProSim Diagram]

- MoT
- ProSim
- Simulis thermodynamic
- ProSim Plus
Computer Aided Process Engineering Tools

1. MoT

2. ProSim
   - Simulis thermodynamics
   - ProSimPlus
   - CO-wrapper
MoT-ProSim Integration

CAPE-OPEN Wrapper
Unit/Thermo
MoT-ProSim Integration

CAPE-OPEN
Wrapper
Unit/Thermo
MoT
ProSim
CO-thermo interface
1. Highlights interoperability through the use of an external model (PC-SAFT) through the CO-thermo interface in ProSim, which is run from EXCEL - for a binary mixture of methane/n-butane (saturation point & property calculations)

2. Highlights interoperability through the use of an external unit operation model (short-path evaporation) for the recovery of a chemical from a feed mixture using ProSim as the simulator and wrapping the MoT-model object for the CO-socket in ProSim
Case Study: PC-SAFT EOS

```plaintext
/* zetas[n] abbreviation |k = 0.3|, |k<=0| */
/* a01, a02, a03 model constant */
/* b01, b02, b03 model constant */
/* RGAS Universal gas constant, [J/(mol K)] */
/* NAV Avogadro's number, [molecules/mole] */
/* kboltz Boltzmann constant, [J/K] = RGAS/NAV */
/* NAV Avogadro's number, [molecules/mole] */
/* PI PI number = acos(-1) */
/* The mixture Butane-Methane is considered as a test system.* */

/* The model */
/* segment diameter of component 1 */
/* d=[1] = sigma[1](1 - 0.13*exp(-3*epsilon[0]*k[1]/T[1]) */

/* segment diameter */
/* d([0]*[1]) = d_0*d[1]/(d_0 + d[1]) */
/* d([1]*[1]) = d_1*d[1]/(d_1 + d[1]) */

/* Combining rules for a pair of unlike segments */
/* sigma([0]*[1]) = 0.5*(sigma_0 + sigma[1]) */
/* sigma([1]*[1]) = 0.5*(sigma_1 + sigma[1]) */
/* epsilon([0]*[1]) = sqrt(epsilon_0*epsilon[k]*epsilon[1]) */
```

AIChe Annual Meeting 2006 - San Francisco California
Case Study: PC-SAFT EOS
Case Study: PC-SAFT EOS
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)

![Image of CAPE-OPEN Thermodynamic Property Package]

<table>
<thead>
<tr>
<th>Name</th>
<th>PCS alt by CAPEC and ProSim</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
<td>CAPE-OPEN Property Package: PCS alt by CAPEC wrapped by ProSim</td>
</tr>
<tr>
<td>ClassID</td>
<td>8BD6D786-9798-486A-A62D-D1A5677CE6B</td>
</tr>
<tr>
<td>ProgID</td>
<td>PCS alt PPI100</td>
</tr>
<tr>
<td>InProcServer32</td>
<td>C:\ProSim\PCSAFT\prosail.dll</td>
</tr>
<tr>
<td>Short description</td>
<td>PCS alt by CAPEC and ProSim</td>
</tr>
<tr>
<td>Full description</td>
<td>CAPE-OPEN Property Package: PCS alt by CAPEC wrapped by ProSim</td>
</tr>
<tr>
<td>Version</td>
<td>1.0.0.0</td>
</tr>
<tr>
<td>About</td>
<td>CAPE-OPEN version 1.0</td>
</tr>
<tr>
<td>Compounds list</td>
<td>n-BUTANE / 106-97-8 / C4H10, METHANE / 74-85-0 / CH4</td>
</tr>
<tr>
<td>Properties list</td>
<td>FugacityCoefficient, density</td>
</tr>
<tr>
<td>Phases list</td>
<td>Vapor, Liquid, VaporLiquid</td>
</tr>
</tbody>
</table>
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)
Case Study 1: Thermo Interface

1. Validation & comparison of results

Fugacity coefficient for n-butane (Liquid phase)

Fugacity coefficient for methane (Liquid phase)

- Simulis (SRK)
- Mot-Prosim (PC-SAFT)
Case Study 1: Thermo Interface

1. Validation & comparison of results

Bubble and Dew point for methane

Temperature:

\[ T = 21.1 \, ^\circ\text{C} \]

Mole fractions:

\[ x_{n-but} = 0.999 \]
\[ x_{CH_4} = 0.001 \]
Short-Path Evaporator Model

Momentum balance

\[ \nu \frac{\partial^2 v(y, z)}{\partial y^2} = -g \]

Rate of Evaporation

\[ \frac{\partial l_i(z)}{\partial z} = -2\pi \cdot R \cdot k_i; \quad k_i = \frac{\gamma \rho_{\text{vap}}}{\sqrt{2\pi \rho_{\text{ref}}}} \left( \frac{P}{P_{\text{ref}}} \right)^{1 - (1 - F) \left[ 1 - e^{-\beta(z)} \right]} \]

Energy balance

\[ \nu (y, z) \frac{\partial T(y, z)}{\partial z} = \frac{\lambda}{\rho C_p} \left[ \frac{\partial^2 T(y, z)}{\partial y^2} + \frac{\partial^2 T(y, z)}{\partial z^2} \right] \]

Mass Balance

\[ \nu(y, z) \frac{\partial C_i(y, z)}{\partial z} = D_i \left[ \frac{\partial^2 C_i(y, z)}{\partial y^2} + \frac{\partial^2 C_i(y, z)}{\partial z^2} \right] \]

Case Study 2: Unit Interface
Case Study 2: Unit Interface

Edition of a CAPE-OPEN Component

This window displays some information about a CAPE-OPEN Component

URL Vendor:  http://www.prosim.net
URL Help:  http://www.prosim.net

Name: CAPEC Evaporator
Description: <none>
ClassID: {ABA99055-1FAE-4808-811F-C4256C4D63FF}
ProgID: CAPECEvaporator.COUnit
InProcServer32: V:\stardust\project\capeopen\gani-evaporateur\CAPECEvapoUnit.dll
Short description: CAPEC Evaporator
Full description: CAPEC Evaporator: CAPE-OPEN Unit by ProSim and CAPEC
Version: 1.0.0.0
About: Copyright © 2006 ProSim - CAPEC

Close
Case Study 2: Unit Interface

Thermodynamic calculator editor

Calculator actions and properties
- Calculator Packages
  - Show the package manager...
  - Import a package...
  - Build a package...
  - Select a CAPE-OPEN package

Modifications:
- Undo
- Redo

Services:
- Calculate
- Export as a PSF file

Name:
- JUNONENE / WATER

Comments:

CAPE-OPEN

Compounds actions
- Edit
  - Import compounds...
  - Edit this compound...
  - Add a new compound
  - Delete the selection
  - Done this compound
  - Create pseudo-compounds...
  - Temperature dependent properties...

Order
- Move this compound up
- Move this compound down

Compounds Packages
- Show the package manager...
- Import a package...
- Build a package with this list...

Comments:

Compounds | Model | Parameter
-----------|-------|----------------

Ok | Cancel
Case Study 2: Unit Interface

The image displays a software interface for configuring a unit operation in a simulation tool. The interface includes sections for identifying process feed, specifying temperature and pressure, and configuring flowrate specifications.

- **Process feed ($ALIM3)**
  - Name: Process feed 1
  - Description: Blank

- **Temperature and Pressure**
  - Pressure specification:
    - Supplied
    - Bubble point pressure at specified temperature
    - Dew point pressure at specified temperature
  - Pressure: 299.02 Pa

- **Flowrate specification**
  - Stream physical state: Liquid stream
  - Enthalpy: 0.00000 cal/mol

The interface provides options for linking data and adjusting parameters to simulate unit operations accurately.
Case Study 2: Unit Interface

CAPEC-OPEN Unit Operation

Name: CAPEC Evaporator
Desc: 

Identification | Parameters | Scripts | Notes |
---|---|---|---|
Specifications management

- **Edit...** Open the edition window of the unit operation in order to visualize or to modify its parameters.
- **Details...** Visualize the registered details of the unit operation on your computer.
- **Parameters...** Open the edition window of the unit operation supplied by Simulis.
- **Validate** Manually start the validation of the unit operation.
- **Reports...** Visualize the reports supplied by the unit operation.

The grayed buttons correspond to actions which are not available or which are not implemented by the unit operation.

OK | Cancel
Case Study 2: Unit Interface

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Type</th>
<th>Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>Evaporator Length (m)</td>
<td>Real</td>
<td>Input</td>
</tr>
<tr>
<td>Diameter</td>
<td>Evaporator Diameter (m)</td>
<td>Real</td>
<td>Input</td>
</tr>
</tbody>
</table>

Value: 0.15
Case Study 2: Unit Interface
Case Study 2: Unit Interface
## Case Study 2: Unit Interface

### 2. Short-Path Evaporator Model

<table>
<thead>
<tr>
<th>Streams</th>
<th>Liaison 1</th>
<th>Liaison 2</th>
<th>Liaison 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>From</td>
<td>Entrée du procédé 1</td>
<td>CAPEC Evaporator</td>
<td>CAPEC Evaporator</td>
</tr>
<tr>
<td>Partial flows</td>
<td>kg/h</td>
<td>kg/h</td>
<td>kg/h</td>
</tr>
<tr>
<td>d-LIMONENE</td>
<td>13.7323872</td>
<td>0.013962354</td>
<td>13.71842485</td>
</tr>
<tr>
<td>WATER</td>
<td>3.63188448</td>
<td>0.109261291</td>
<td>3.522623189</td>
</tr>
<tr>
<td>Partial flows</td>
<td>mol/s</td>
<td>mol/s</td>
<td>mol/s</td>
</tr>
<tr>
<td>d-LIMONENE</td>
<td>0.028</td>
<td>2.84689E-05</td>
<td>0.027971531</td>
</tr>
<tr>
<td>WATER</td>
<td>0.056</td>
<td>0.001684699</td>
<td>0.054315301</td>
</tr>
<tr>
<td>Total flow</td>
<td>kg/h</td>
<td>17.36427168</td>
<td>0.123223645</td>
</tr>
<tr>
<td>Physical state</td>
<td>Vapor</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Temperature</td>
<td>K</td>
<td>363</td>
<td>350.8500852</td>
</tr>
<tr>
<td>Pressure</td>
<td>Pa</td>
<td>299.0199192</td>
<td>299.0199192</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>kcal/h</td>
<td>431.2384293</td>
<td>5.53628E-05</td>
</tr>
</tbody>
</table>

---

**CAPEC Evaporator**

**Liaison 1**

**Liaison 2**

**Liaison 3**

**Streams**

**Partial flows**

**d-LIMONENE**

**WATER**

**Total flow**

**Physical state**

**Temperature**

**Pressure**

**Enthalpy**
Conclusions

- Through two (MoT & ProSimPlus) modelling/simulation tools, it has been shown how to apply the CO-interfaces with few additional programming effort.
- Using the highlighted approach, any new thermo-model or unit operation model can be converted into a model object, which is then connected to a simulation environment supporting CO-interfaces, thereby achieving plug & play (interoperability) of software tools and models.
- Current and future work is extending this approach to other modelling problems, such as, parameter estimation, customized simulators, and modelling for product behaviour analysis.