

ProSimPlus



New CAPE-OPEN capabilities

#535b – CAPE-OPEN Unit Operations: Development and Usage (TD001)

Alain VACHER, Stéphane DECHELOTTE, Olivier BAUDOUIN



ProSim SA

Stratège Bâtiment A
BP 2738
31312 LABEGE Cedex
FRANCE
www.prosim.net
info@prosim.net

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 - CO-SPEC: a CAPE-OPEN Unit implementation
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CAPE-OPEN Thermodynamic Socket



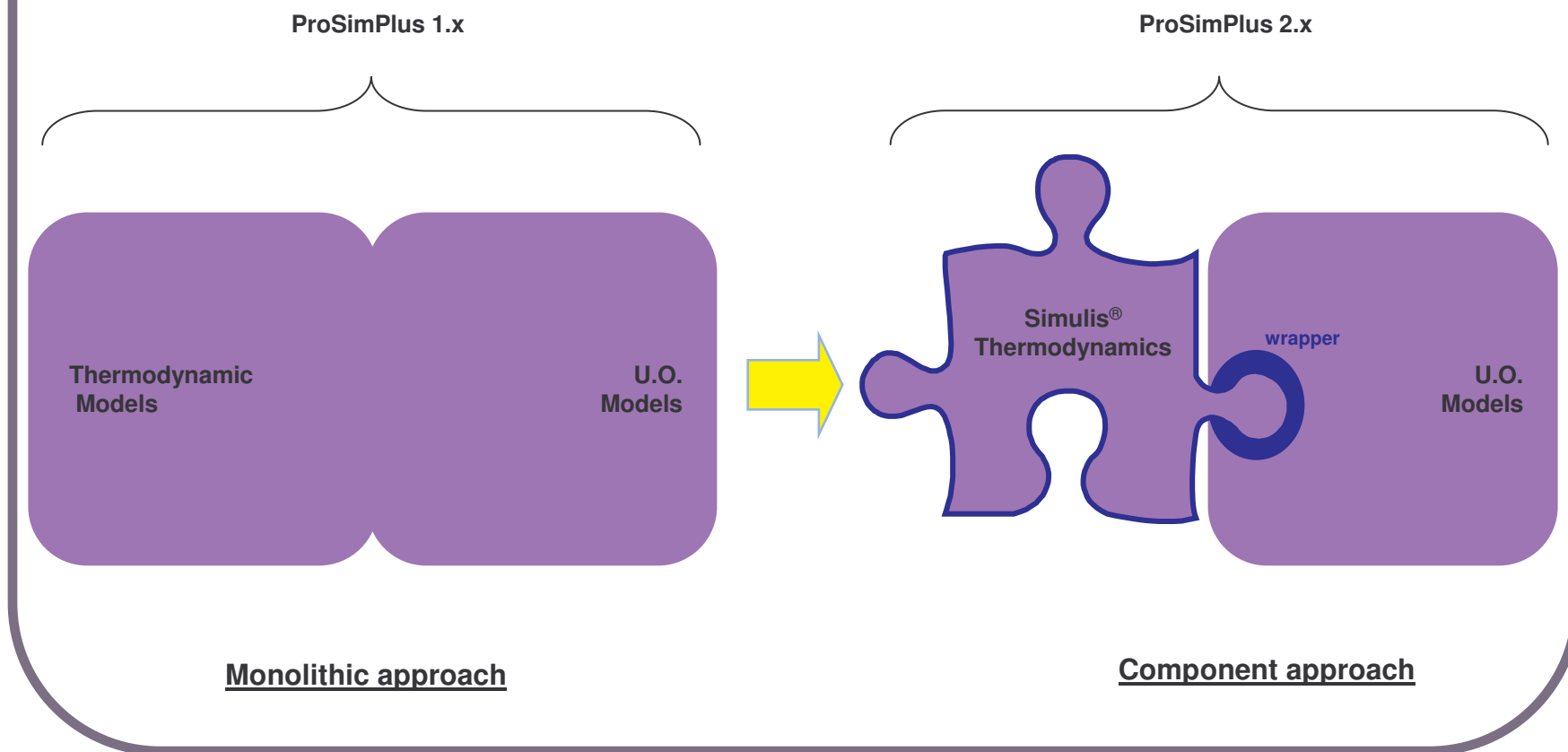
- Capability to use a third-party thermodynamic package
- Our manner to provide it:
 - A constraint:
 - minimize the modifications of the existing code
 - A solution:
 - write of a wrapper of Simulis[®] Thermodynamics



CAPE-OPEN Thermodynamic Socket



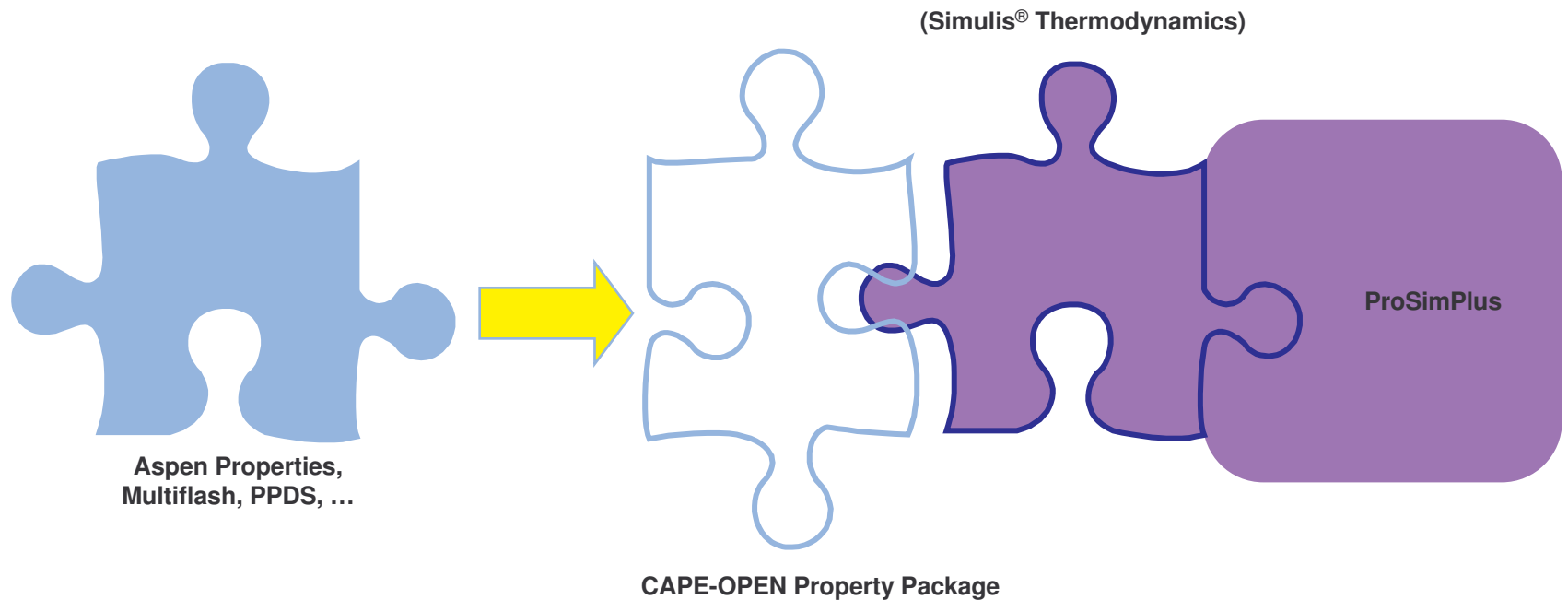
- Wrapping of Simulis Thermodynamics:



CAPE-OPEN Thermodynamic Socket



- An additional benefit of Simulis Thermodynamics



CAPE-OPEN Thermodynamic Socket

The screenshot displays the ProSim Plus interface with several overlapping windows. The main window is titled "ProSim Plus : Unnamed.pmp" and shows a menu bar (File, Edit, Configuration, Flowsheet, Tools, Simulation, Windows, Help) and a toolbar. A sidebar on the left lists various process units like "Absorbers", "Feed/P...", "Mas...", "2-ph...", "3-phase distillation", "Heat exchangers", "Liquid-liquid extraction", "Flashes and decanters", "Compressor/Expander/Pump", "Mixers / Splitters / Separators", "User defined unit operations", "Reactors", and "Liquid-solid separation".

Overlaid on the main window are three windows related to thermodynamic calculations:

- Thermodynamic calculators editor**: Shows "Calculator Packages" with options like "Show the package manager...", "Import a package...", "Build a package...", and "Select a CAPE-OPEN package". It also has "Modifications" (Undo, Redo) and "Services" (Calculate, Export as a PSF).
- Selection of a CAPE-OPEN Thermodynamic Property Package**: A list box showing various packages. The "CAPE-OPEN" package is selected. Below the list, it says "This window allows to select a Thermodynamic Property Package. Double-click on an item to select it." The list includes:
 - RSI/PDST ThermoSystem**
 - Simulis CAPE-OPEN[®] Thermo System** (italicized):
 - Water/Ethanol/FLU 2006
 - Water/Ethanol with NRTL
 - Sourwater-NaOH
 - HYP/SRK ThermoSystem**:
 - COPropPack.COPropPack
 - HDAPPack.HDAPPack
 - HyHDAPPack.HypHDAPPack.1
 - ThermoPack Class**:
 - C1_C2
 - C1_C2 (EOS)
 - n-deopropanizer
 - alkanes
 - HDA
 - Water
 - Water Bis
 - C1 - C2 (Test1.1)
- Edition of a CAPE-OPEN Thermodynamic Property Package**: A form for editing the selected package. It contains:
 - CAPE-OPEN** header with a note: "This window displays some information about a CAPE-OPEN Thermodynamic Property Package".
 - URL Vendor: <http://www.cocosimulator.org/>
 - URL Help: [<none>](#)
 - Fields for Name (Water), Description (Pure Water Package), ClassID (90DAC7FA-E0E4-40B5-A903-E0B12774D52B), ProgID (COCCD_TEA.ThermoPack.1), InProcServer32 (C:\Program Files\COCCD\COCCDTEA.dll), Short description (TEA (CAPE-OPEN 1.0)), and Full description (COCCD Thermodynamics for Engineering Applications).
 - Version (1.0) and CAPE-OPEN version (1.0).
 - About text: Cape Open 1.0 Thermo Package - Copyright 2006 cocosimulator.org
 - Three lists: Compounds list (Water / 7732-18-5 / HOH), Properties list (activity.Dmoles, activity.DmolesFraction, activity.Dpressure, activity.Dtemperature, activity.Coefficient, activity.Coefficient.Dmoles), and Phases list (Overall, Vapor, Liquid).
 - Buttons for "Close", "Select", and "Cancel".

CAPE-OPEN Unit Socket



- Capability to use a third-party unit operation
- Development easy to do with the help of...
 - ... previous integration of Simulis Thermodynamics
 - Each calculator is a Material Object Template
 - ... creation of Material Objects (material streams)
 - CAPE-OPEN Thermodynamic Socket is available
 - ... existing event handler within ProSimPlus





- Event handling

- Simulation level:

- OnSimulationStart

- "validate" call

- OnSimulationEnd

- integration of U.O. reports in the simulation report (not yet done)

- Unit operation level (... useful for iterative processes):

- OnCalculationStart

- mapping of input material and information objects

- OnCalculation

- "calculate" call

- OnCalculationEnd

- mapping of output material and information objects



CAPE-OPEN Unit Socket



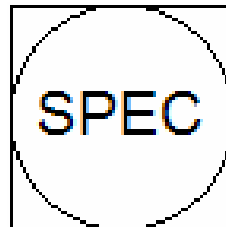
The screenshot displays the ProSim Plus interface with a 'Selection of a CAPE-OPEN Component' dialog box open. The dialog lists various unit operation classes, with 'HtriCD100.Xist' selected. In the background, the 'HTRI Xchanger Suite v5.00' window is visible, showing the 'Input Summary' tab. The 'Case Mode' is set to 'Rating'. The 'Exchanger Configuration' section shows 'Generic Shell and Tube' selected. The 'Process Conditions' section includes fields for Flow rate, Inlet/outlet Y, Inlet/outlet T, Inlet P/allow dP, and Fouling resistance. The 'Shell Geometry' section includes TEMA type (A, E, S), ID, Orientation, and Hot fluid. The 'Baffle Geometry' section includes Type (Single segmental), Orientation, Cut, and Spacing. The 'Tube Geometry' section includes Type (Plain), Wall thickness, Length, Layout angle, Tube OD, Tubepasses, Pitch, and Tubecount. The 'HTRI Xchanger Suite v5.00' window also shows a 'For Help, press F1' message and 'Select' and 'Cancel' buttons.



Other CAPE-OPEN aspects



- A CAPE-OPEN Unit Socket but also...



- ... a CAPE-OPEN Unit implementation: CO-SPEC
 - Same model as the SPEC module of ProSimPlus
 - solve material recycles
 - solve design specifications
 - CAPE-OPEN Unit Object \neq CAPE-OPEN Solver Object
 - Clearly a non conventional unit operation
 - bring powerful solving capabilities within simulators lacking such capabilities
 - CO-SPEC needed:
 - extension to CAPE-OPEN standards
 - specific requirements related to the communication with the simulator



Other CAPE-OPEN aspects



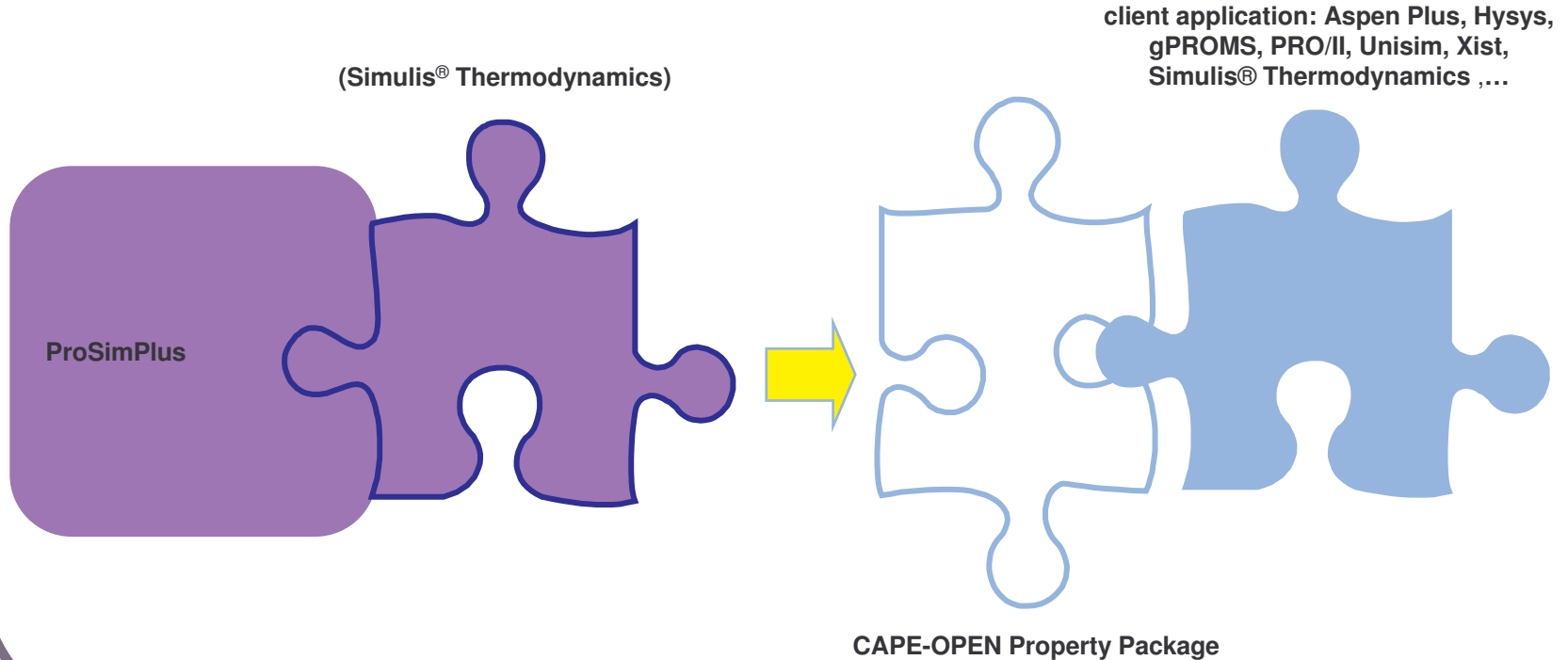
- CO-SPEC: CAPE-OPEN extension
 - Management of design specifications:
 - use of information streams
 - specification: input information of CO-SPEC
 - action variable: output information of CO-SPEC
 - information object → CAPE-OPEN Real Parameter
- Specific requirements between CO-SPEC and the simulator
 - Maximal Cyclic Network (MCN) marks:
 - identify the number and the order of unit operations
 - the calculation list of unit operations is provided "manually"
 - Convergence flag
 - a compulsory CAPE-OPEN Boolean Parameter
 - stop the calculation sequence (iterative process)



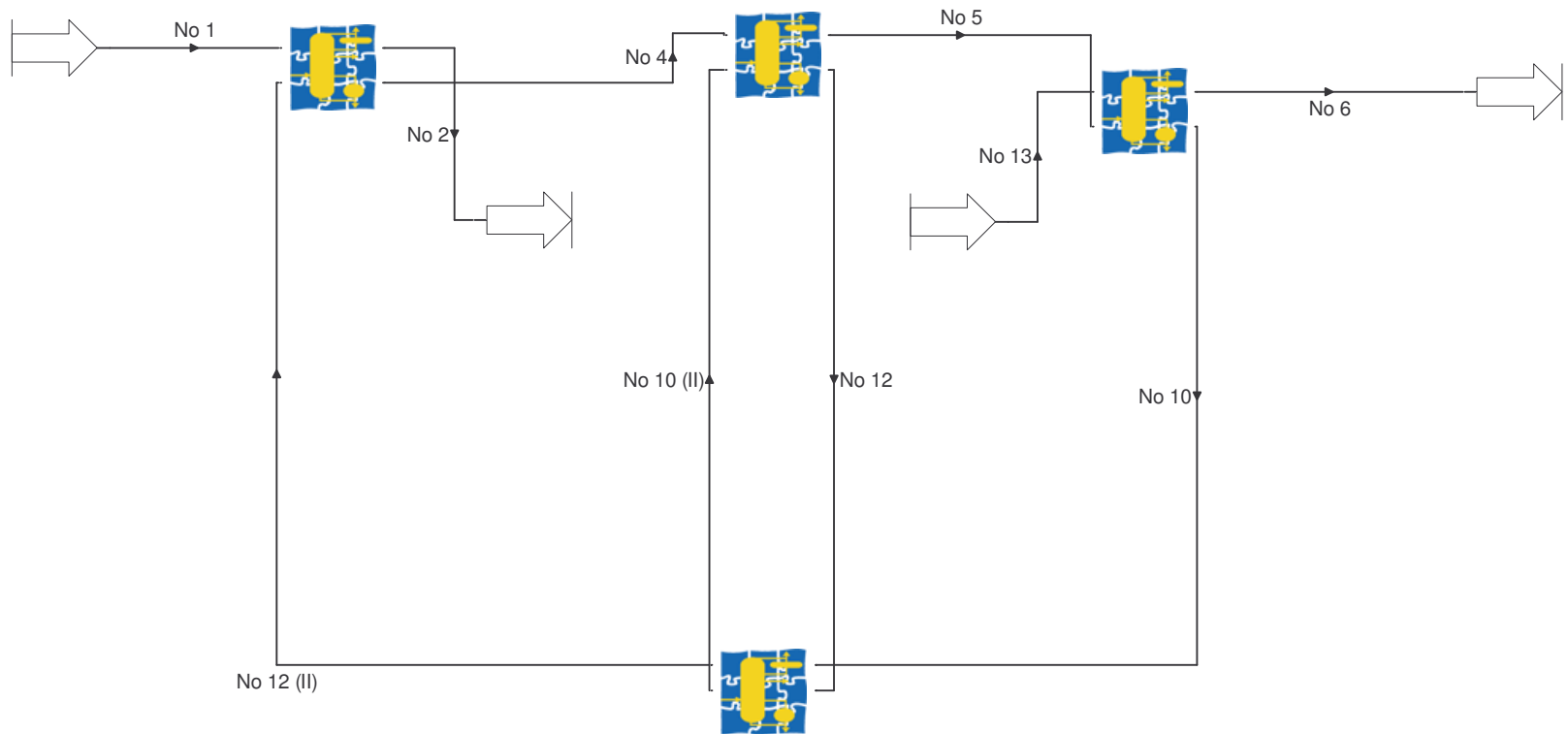
Other CAPE-OPEN aspects



- Another benefit of Simulis Thermodynamics:
 - CAPE-OPEN Thermodynamic Plug



Assembly of components



Conclusion & Perspectives



- Increase the openness of the simulator
 - external thermodynamic package
 - external unit operation
- A few comments from our experience:
 - Not really a long development
 - but a long test period
 - Loss of performance
 - depends on the quality of software components



Conclusion & Perspectives



- Successful tests:
 - CAPE-OPEN Thermodynamic Socket
 - Aspen Properties (Aspentech)
 - COM Thermo (Aspentech)
 - MultiFlash (Infochem)
 - PPDS (TÜV NEL)
 - COCO TEA (AmsterCHEM)
 - CAPE-OPEN Unit Socket
 - Xist, Xphe... (HTRI)
 - COCO-COUSCOUS (AmsterCHEM)
 - ChemSep (ChemSep)
- Further interoperability situations to be checked:
 - IFP Pipe, SolidSim...



ProSimPlus



New CAPE-OPEN capabilities
... thanks you for your attention...



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