

Simulis[®] Thermodynamics



Use of a CAPE-OPEN Thermodynamic Server in Legacy Codes

#580a – CAPE-OPEN Compliant Thermodynamic Components (TD002)

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Introduction



- Objective
 - Perform easily calls to a CAPE-OPEN Thermodynamic Property Package in legacy codes throughout the thermodynamic server Simulis® Thermodynamics
 - Provide a solution independent of the legacy code programming language

- Example written in Visual Basic 6.0
 - requested calculations:
 - TP flash
 - liquid and vapor composition
 - equilibrium constants
 - For each phase:
 - Molecular weight
 - Dynamic viscosity
 - Thermal conductivity





- **Is a thermodynamic calculation server**
 - **A major element of our new software component suite**
 - other components: unit conversions, pure compound properties
 - **Based on a component-oriented approach**
 - COM middleware
 - **Created by wrapping of our existing well-proven codes**
 - efficiency, reliability, validated code
 - **Required a client application to be executed**
 - Microsoft Excel, MATLAB...
 - **Easily integrated within a client application**
 - Visual C++, Visual Basic, Delphi, C#... even FORTRAN





- **Thermodynamic properties and phase equilibrium calculation server (max. 200 compounds)**
 - **Properties and derivatives**
 - Transport properties (C_p , C_v , μ , λ , ...),
 - Thermodynamic properties (H , S , U , ...),
 - Compressibility properties (Z , C_p/C_v , ...),
 - Non-ideal properties (γ , ϕ , $\ln(\phi)$, ...),
 - Pseudo critical properties (T_c , P_c , V_c , Z_c).
 - **Equilibrium**
 - Liquid-Vapor (TP , HP , SP , ω_T , ω_P , UV , ...),
 - Liquid-Liquid (TP),
 - Liquid-Liquid-Vapor (TP , HP , ω_P),
 - Liquid-Vapor phase envelope,
 - Liquid-Vapor equilibrium constants and derivatives,
 - Liquid-Liquid equilibrium constants and derivatives.





- **Thermodynamic models**

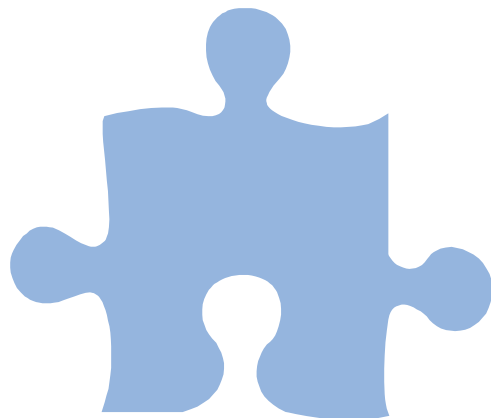
- Soave-Redlich-Kwong (SRK),
- Peng-Robinson (PR),
- Lee-Kesler-Plöcker (LKP),
- Benedict-Webb-Rubin modified Starling (BWRS),
- Ideal,
- Wilson,
- NRTL,
- Margules,
- UNIQUAC,
- UNIFAC original,
- UNIFAC modified Dortmund,
- UNIFAC modified Larsen,
- PSRK,
- UNIFAC LL,
- Engels,
- Chao-Seader,
- Sour water,
- Amines and acid gases,
- MHV2,
- ULPDHS...



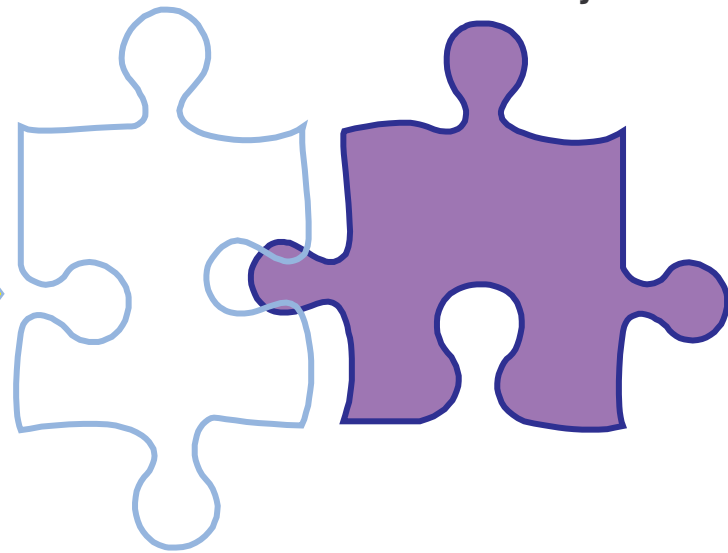
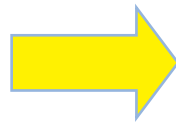
CAPE-OPEN and Simulis® Thermodynamics

● CAPE-OPEN Thermo Socket

- use of a third-party thermodynamic package
- successfully checked with:
 - Aspen Properties (AspenTech)
 - MultiFlash (Infochem)
 - PPDS (TÜV NEL)
 - COCO TEA (AmsterCHEM)



Aspen Properties,
Multiflash, PPDS, ...



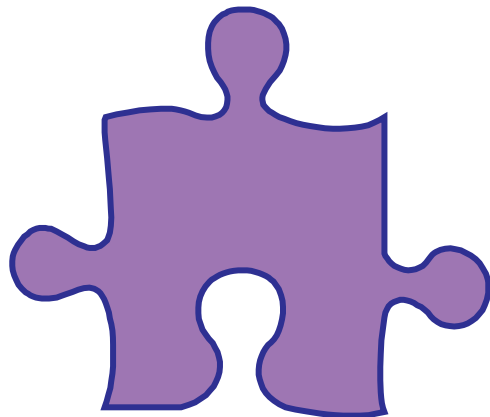
CAPE-OPEN Property Package



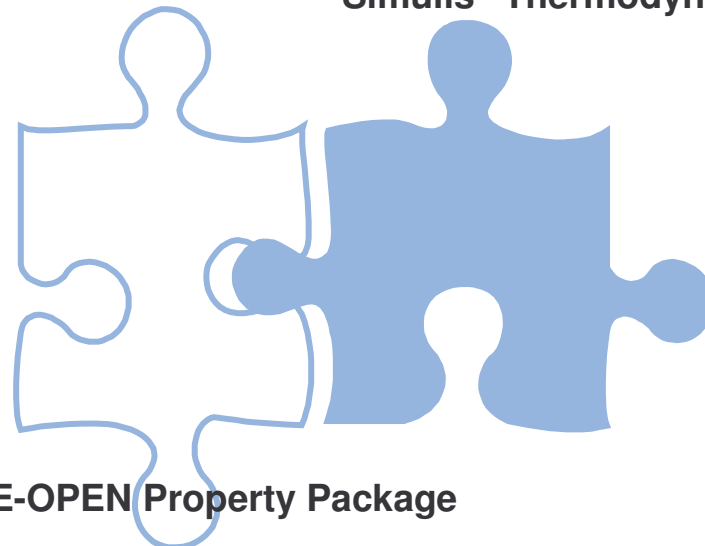
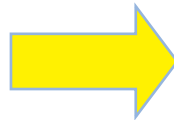
CAPE-OPEN and Simulis[®] Thermodynamics

● CAPE-OPEN Thermo Plug

- creation of a thermodynamic package
- successfully checked with:
 - Aspen Plus, Aspen Hysys (AspenTech)
 - PRO/II (SimSci)
 - gPROMS (PSE)
 - Xist,... (HTRI)
 - Unisim (Honeywell)
 - INDISS (RSI)
 - COCO COFE (AmsterCHEM)



Simulis[®] Thermodynamics



CAPE-OPEN Property Package

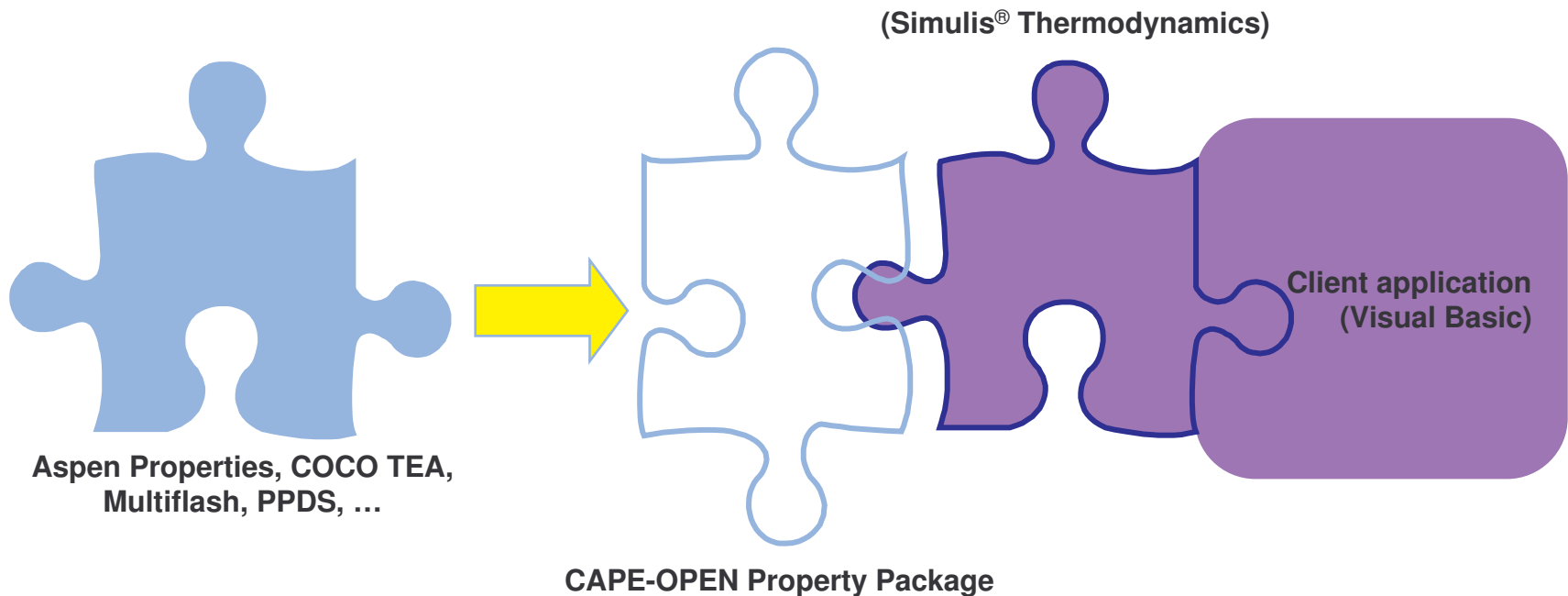
Aspen Plus, Hysys,
gPROMS, PRO/II, Unisim, Xist,
Simulis[®] Thermodynamics ,...



An example using Visual Basic



- Architecture view of example presented



An example using Visual Basic

The image shows a screenshot of the Microsoft Visual Basic IDE. A 'Nouveau projet' (New Project) dialog box is open in the foreground, displaying various project templates such as 'EXE standard', 'EXE ActiveX', 'DLL ActiveX', 'Contrôle ActiveX', 'Assistant Création d...', 'Gestionnaire d'Assistants', 'Addin', 'Application DHTML', 'Application IIS', 'Contrôles de VB Édition...', 'DLL Document ActiveX', and 'EXE Docum...'. The 'Ouvrir' (Open) button is highlighted. In the background, the Visual Basic IDE is visible, showing a code editor window with the following code:

```
Project1 - Microsoft Visual Basic [création] - [Form1 (Code)]
Echier Edition Affichage Projet Format Débogage Exécution Requête Schéma Outils Compléments Fenêtre 2
Ln 30, Col 18

MolFractions(0), _
sInit(0), yMolFractionsInit(0), _
ctions(0), eConstants(0))

6 " K")
atm")

rVapRatio))

lFractions(i) & " yv=" & yMolFractions(i) & _

Calc, xMolFractions(0))

olFractions(0))

Calc, xMolFractions(0))
```

Below the code editor, a snippet of code is visible:

```
mVL = 0#
mUL = 0#
lambdaL = 0#
End If
' calculations of properties related to the vapor phase
If (molarVapRatio > 0#) Then
mV = calcObject.FCalcExtendedMwV(temperatureCalc, pressureCalc, yMolFractions(0))
Call calcObject.CheckPureProperties(208, 1, iError)
```



Conclusions and perspectives



● Benefits

○ Reduction of costs

● Reduction of development time

- no knowledge of CAPE-OPEN technology is required

● Reduction of training time

- same API (developers), same GUI (end-users)

○ Different available languages

● C++, Visual Basic, C#... even FORTRAN

○ CAPE-OPEN socket and our native calculation library

○ Thermodynamic consistency in all your applications

● CAPE-OPEN Thermodynamic version 1.1 (early 2007)

○ Socket and Plug support



Simulis[®] Thermodynamics



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... thank you for your attention...



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