

Interoperability
Experiments on
MATLAB® / Simulis®



Thermodynamics / COCO TEA
via CAPE-OPEN standard.
Application to ternary liquid-vapor
equilibrium representations.



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OUTLINE



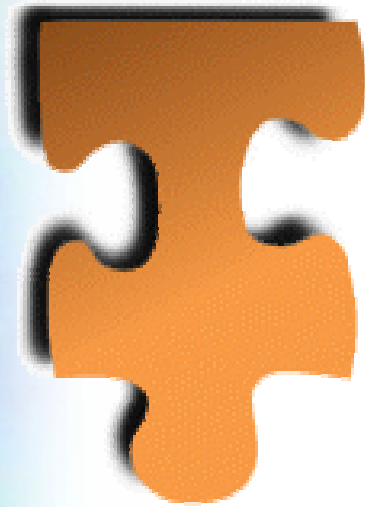
- 3D LV equilibrium representation
- « Third part » architecture Matlab[®] / Simulis[®] Thermodynamics / Coco Tea Demo
- Conclusion and perspectives

3D LV equilibrium representation



- It is a good way to visualize residue curves map for two-phase three-component mixtures
- Singular points (saddle point, minima, maxima) are easily understanding on 3D graphs or 2D contours
- Matlab[®] has good graphical tools, but no thermodynamics capabilities
- Thermodynamics equilibria are calculated by CO property package (here COCO TEA) by the way of CO sockets of Simulis[®] Thermodynamics

Third Part Architecture



CO Property
Package
COCO TEA



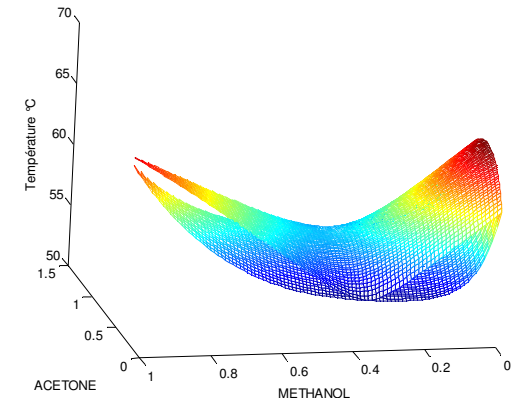
CO Thermo Socket



Simulis®

Matlab®

Thermodynamics Application



First Step : Property Package Creation COCO TEA



TEA Thermo: Property pack templates:

- C1_C2
- C1_C2 (EOS)
- n-depropanizer
- alkanes
- HDA
- Water-nB
- MeOH-Et
- Acetone-t

Buttons: Create template, Edit template

Property pack definition:

Property	Overall	Vapor	Liquid	VaporLiquid
Equation of state		Ideal gas law	N/A	
activityCoefficient	N/A	N/A	NRTL	N/A
enthalpy	SumOfP...	EOS	Ideal+Excess	N/A
excessEnthalpy	N/A	N/A	From activity coefficient	N/A
heatOfVaporization	Pitzer			
logFugacityCoefficient	N/A	EOS	From activity coefficient	N/A
vaporPressure	LeeKesler			
volume	SumOfP...	EOS	Rackett	N/A

Buttons: Add property, Delete property

Buttons: Help, Check, Load, OK, Cancel

Checkboxes: Only show equilibrium phases

Second Step : Client Application Development + Simulis[®] Thermo Plug



The screenshot displays the MATLAB environment with the following components:

- Editor:** A function file named `Equilibre_LV.m` is open. The code includes a function definition, comments, and logic for handling user input and calculating equilibrium properties using Simulis Thermo plug-ins.
- Command Window:** Shows the execution of the `Equilibre_LV` function, with output for composition variables `Z1` and `Z2`.
- Command History:** Lists previous commands and their execution times, including `Solubilite`, `Equilibre_LV`, and `Equilibre_LV`.

```
function [] = Equilibre_LV(cmd);
% GUI for calculating and 3D displaying
% LV equilibria.
% Pascal FLOQUET - ENSIACET - 2005
% TD 3A CAP
% usage : Equilibre_LV

% Flag Programming
if nargin == 0
    Equilibre_LV_init; % Gui Initialization
else
    h = get(gcf,'userdata'); % Handles Recuperation
    switch cmd
        case 'Choice1'
            Equilibre_LV_choice1(h);
        case 'Choice2'
            Equilibre_LV_choice2(h);
    end
end
```

```
296 = 0;% Output Composition Type(0 = mol, 1 = mass)
297
298 y BubbleTemperature and Dew Temperature Calculations
299 ar during calculation
300 tbar(0,'Please Wait...');
301 N
302 i=1:M
303 if (X1(i,j) + X2(i,j) <= 1)
304     Composition = [X1(i,j) X2(i,j) 1 - X1(i,j) - X2(i,j)];
305     try
306         Z1(i,j) = stCALBubbleTemperature(Calc,Pressure,Composition,Type
307         Z2(i,j) = stCALDewTemperature(Calc,Pressure,Composition,Type_I
308     catch
309         %display('Erreur de calcul');display(X1(i,j));display(X2(i,j))
310         Z1(i,j) = NaN;
311         Z2(i,j) = NaN;
312     end
313 else
314     Z1(i,j) = NaN;
315     Z2(i,j) = NaN;
316 end;
```

Third Step : CAPE-OPEN CO Socket in action



The screenshot displays the MATLAB environment with several windows open:

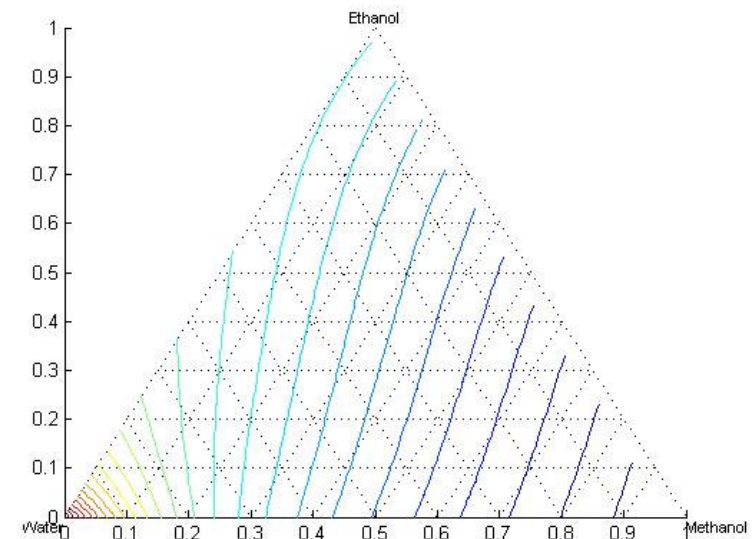
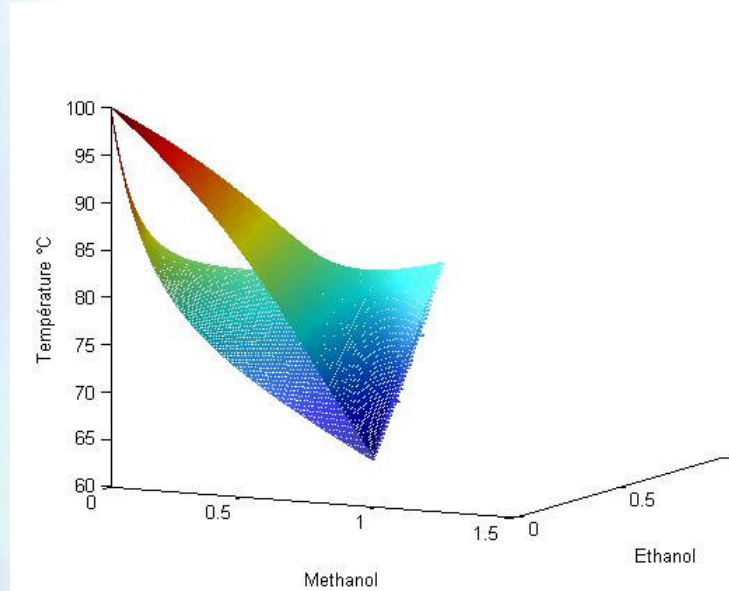
- Equilibre LV:** A window for thermodynamic calculations with fields for "Température de Bulle" and "Triangulaire 3D", and buttons for "Calcul" and "Tracer".
- Editeur de calculator thermodynamique:** A window for configuring the calculator, showing "Actions et propriétés du calculator" and "Modifications".
- Edition d'un CAPE-OPEN Thermodynamic Property Package:** A window for editing the package properties for "MeOH-EtOH-Water".

The **Edition d'un CAPE-OPEN Thermodynamic Property Package** window contains the following information:

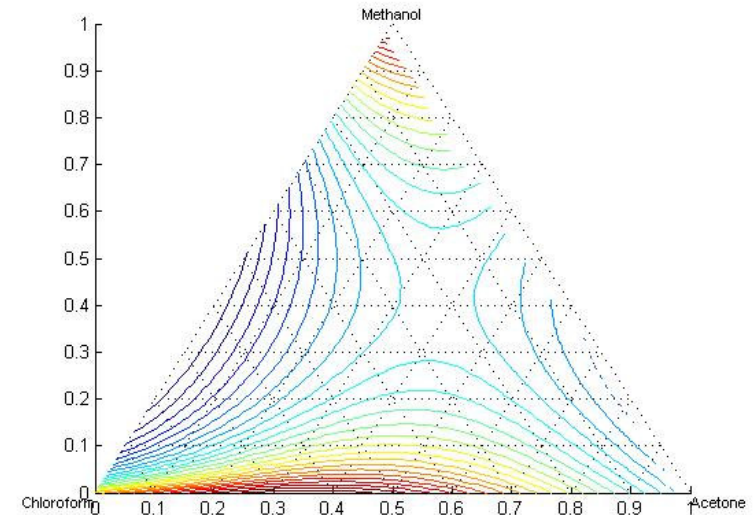
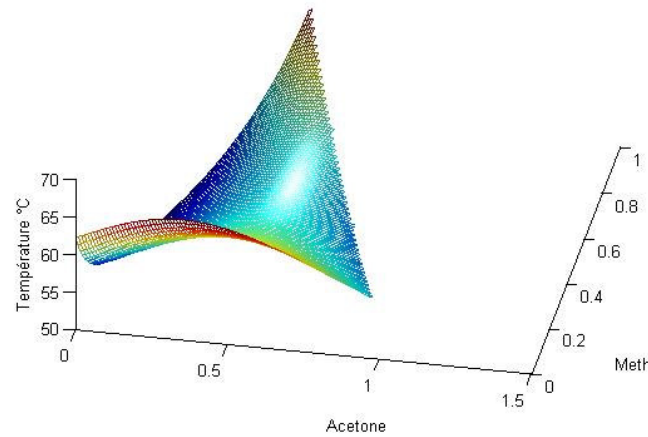
- CAPE-OPEN** (with a small diagram icon)
- URL: <http://www.cocosimulator.org/>
- URL d'aide: [<Aucun>](#)
- Nom:** MeOH-EtOH-Water
- Description:** Methanol/Ethanol/Water mixture NRTL
- ClassID:** {90DAC7FA-E0E4-40B5-A903-E0B12774D52B}
- ProgID:** COCO_TEA.ThermoPack.1
- InProcServer32:** C:\Applications\COCO\COCOTEA.dll
- Description résumée:** TEA (CAPE-OPEN 1.0)
- Description complète:** COCO Thermodynamics for Engineering Applications
- Version:** 1.0 (Version CAPE-OPEN 1.0)
- A propos:** Cape Open 1.0 Thermo Package - Copyright 2006 cocosimulator.org
- Liste de constituants:** Methanol / 67-56-1 / CH3OH, Ethanol / 64-17-5 / CH3CH2OH, Water / 7732-18-5 / H2O
- Liste de propriétés:** activityCoefficient, activityCoefficient.Dmoles, activityCoefficient.DmolFraction, activityCoefficient.Dpressure, activityCoefficient.Dtemperature, enthalpy, enthalpy.Dmoles
- Liste de phases:** Overall, Vapor, Liquid

The bottom of the screen shows the Windows taskbar with the Start button and various application icons including MATLAB, Editor, Equilibre LV, Editeur de c..., Edition d'u..., Boîte de réc..., Z Explorat..., Microsoft P..., http://intra..., TEA Thermo, and Sans titre - ...

Simple Example : Methanol-Ethanol-Water mixture Bubble and Dew Points



Another Example : Acetone-Methanol-Chloroform mixture Bubble Points



Conclusions and perspectives

- Benefits for the user
 - The best tool for the best use
 - MATLAB® development and graphical tool
 - Simulis® Thermodynamics thermodynamic calculation server
 - COCO TEA Property Package
 - Reduction of development time ...even for students
 - No CO Knowledge required : Simulis® Thermodynamics is a good « bridge » between application and CO Property Package
- Something wrong ?
 - Efficiency in terms of CPU time consuming
 - Interoperability of the institutions and licence servers
- Perspectives
 - 3D representation of equilibrium + reaction (reactive residue curve map)
 - Integration of CO Unit Operation in Matlab® application

