Interoperability Experiments on MATLAB® / Simulis® Thermodynamics / COCO TEA *via* CAPE-OPEN standard.

Application to ternary liquid-vapor equilibrium representations.

*Pascal Floquet, Xavier Joulia, Alain Vacher*

le **LABORATOIRE DE GÉNIE CHIMIQUE**
● UMR 5503
TOULOUSE

INP TOULOUSE **ENSIACET** *A7*

ProSim

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
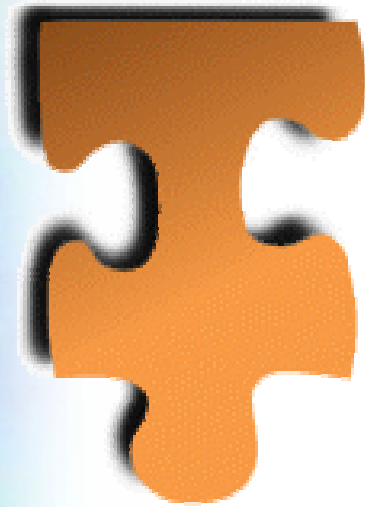
CO Property Package
COCO TEA

CO Thermo Socket

Simulis®
Thermodynamics

Matlab®
Application
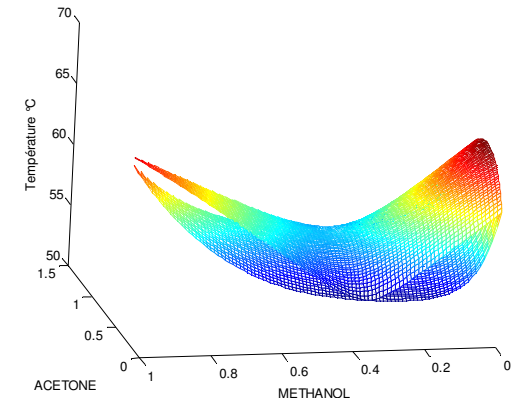
First Step : Property Package Creation COCO TEA

Second Step : Client Application Development + Simulis® Thermo Plug

Third Step : CAPE-OPEN
CO Socket in action

Simple Example : Methanol-Ethanol-Water mixture Bubble and Dew Points
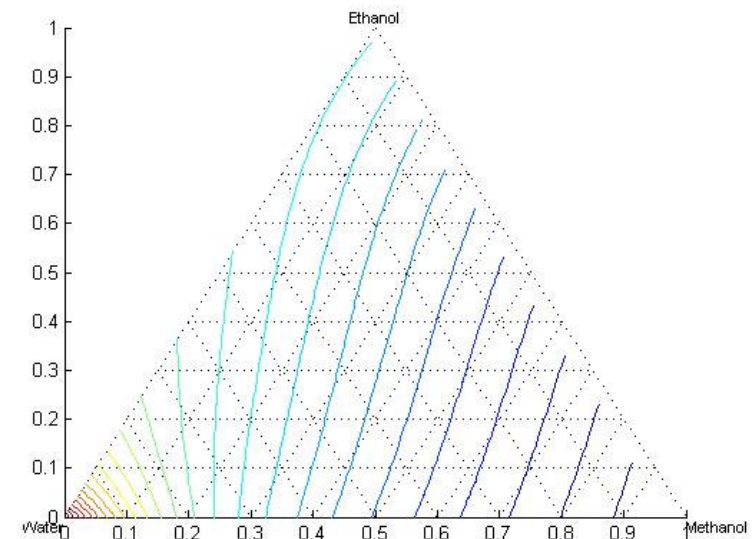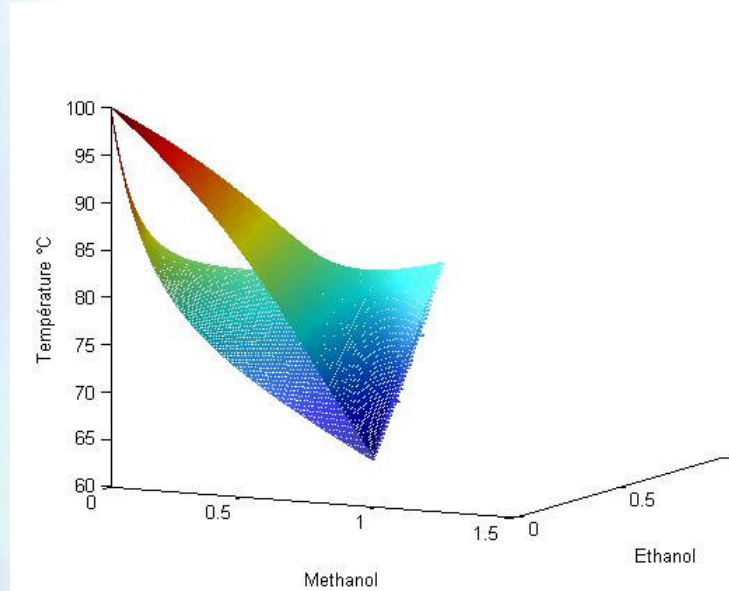
Another Example : Acetone-Methanol-Chloroform mixture Bubble Points
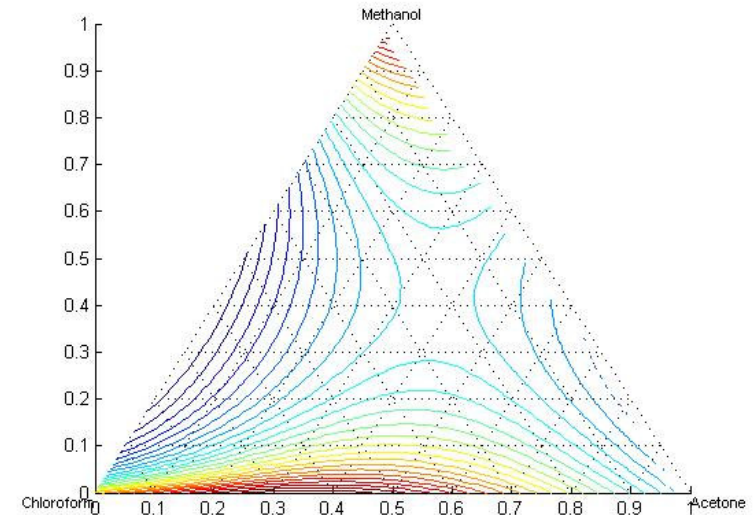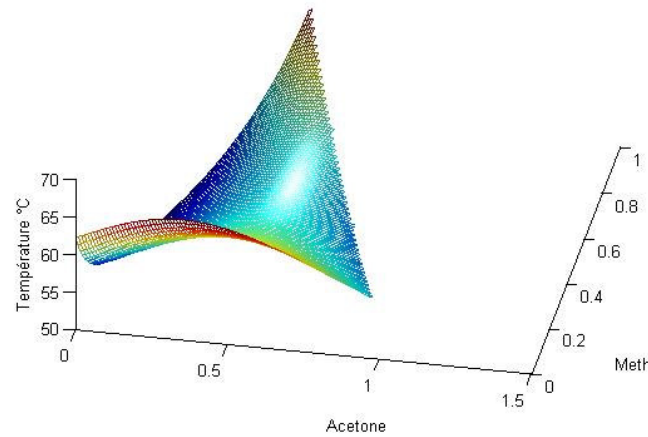
Conclusions and perspectives

- 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