



Air Liquide use of CAPE-OPEN

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- Main actions decided since 2004
- Property package development methodology
- Example of development
- Conclusions and future steps

Main actions decided since 2004

- Participation to CO-LaN as full member

- Adoption of a thermodynamic standard usable at each step of process development (from R&D to Engineering to Plant Operation)
 - Database of pure substances properties: DIPPR from AIChE
 - Server of thermodynamic models and associated resolution algorithms: Simulis Thermodynamics (Prosim SA)
 - Software component for computing thermophysical properties and phase equilibria on pure components or mixtures in MS-Excel (Add-In functions), Matlab® or any CAPE-OPEN Process Modelling Environment

- Development of concept of CAPE-OPEN “thermodynamic property package” dedicated to given applications
 - Interoperability of packages: PMEs (Aspen Hysys, Belsim-Vali, Prosim Plus), Excel®, Matlab®
 - Consistency of results throughout different applications
 - Perpetuation of in-house knowledge: database of packages
 - Detailed description and validity range
 - References of experimental values (literature, in-house)
 - Improvement of accessible information quality for a relevant later re-use

- What is a “Thermodynamic Property Package”?
 - Database of properties of pure compounds
 - Equation of state dedicated to the vapor phase
 - Equation of state or Activity coefficients models dedicated to the liquid phase
 - Mixing rules
 - State reference of enthalpy calculation
 - Algorithm of resolution of phase equilibrium
 - Calculation methods of transport properties (thermal conductivity, viscosity, surface tension)

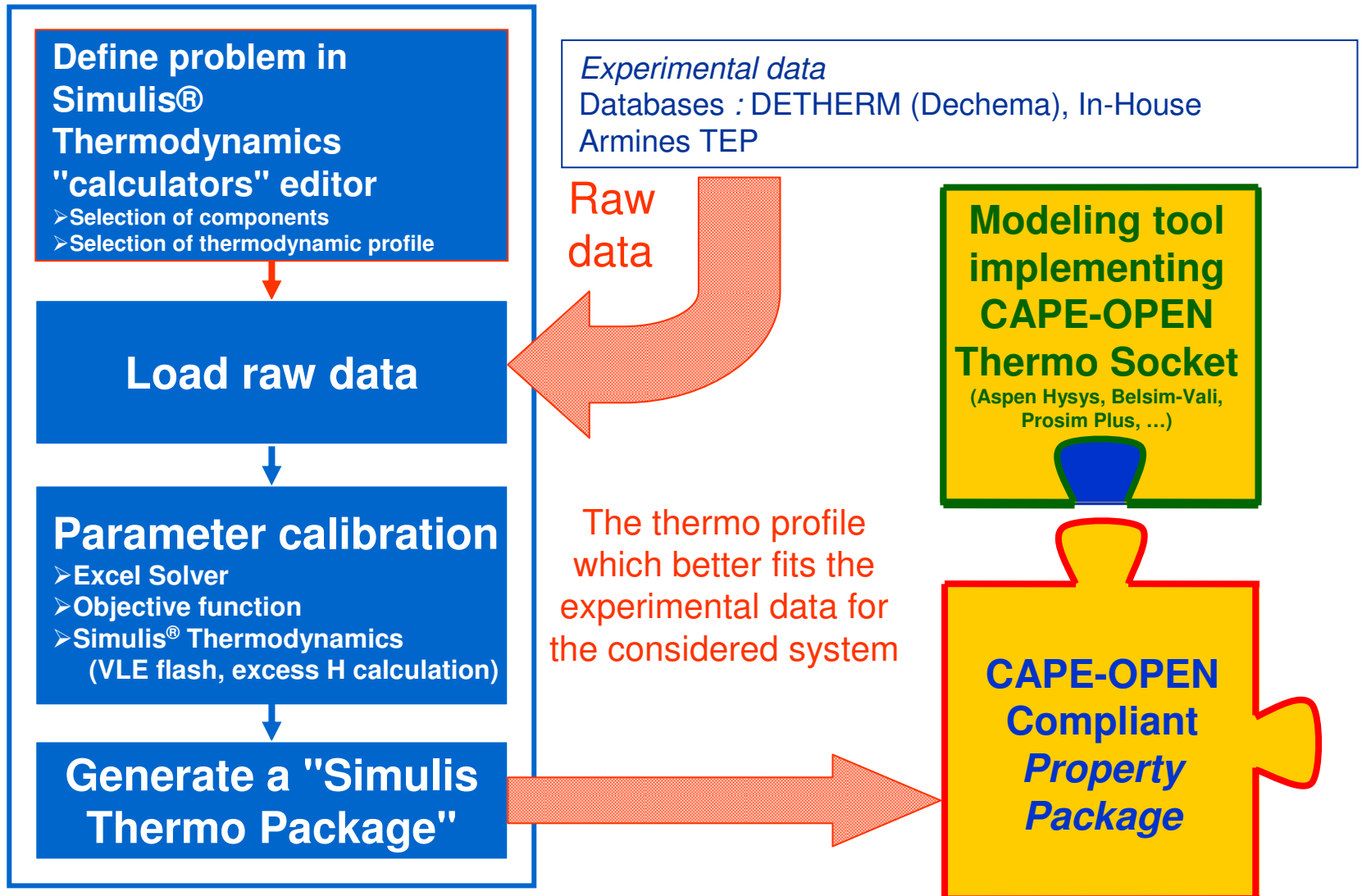
Property package development methodology



- Property package development methodology
 - Bibliographic study (measurements)
 - Choice of a thermodynamic profile
 - Evaluation of calibration requirement, if yes
 - Evaluation of requirement for additional experimental values in studied conditions
 - Question: what is the minimum number of supplementary experimental values to be measured to avoid significant errors?
 - If yes, Campaigns of measurements
 - In-House
 - Partner: Ecole des Mines de Paris, Centre Energétique et Procédés, laboratoire des Equilibres entre Phases (Armines TEP)
 - Calibration of the model
 - Definition of the objective function according to the unit operation to which to Property Package will be dedicated: choice of properties taken into account (liquid and vapor phase composition, excess enthalpy, ...)
 - Binary interaction coefficient linear function according to temperature : yes or not
 - Value of the objective function at convergence
 - Creation of the CAPE-OPEN Property Package
 - Transfer of the property package from R&D to Air Liquide Engineering

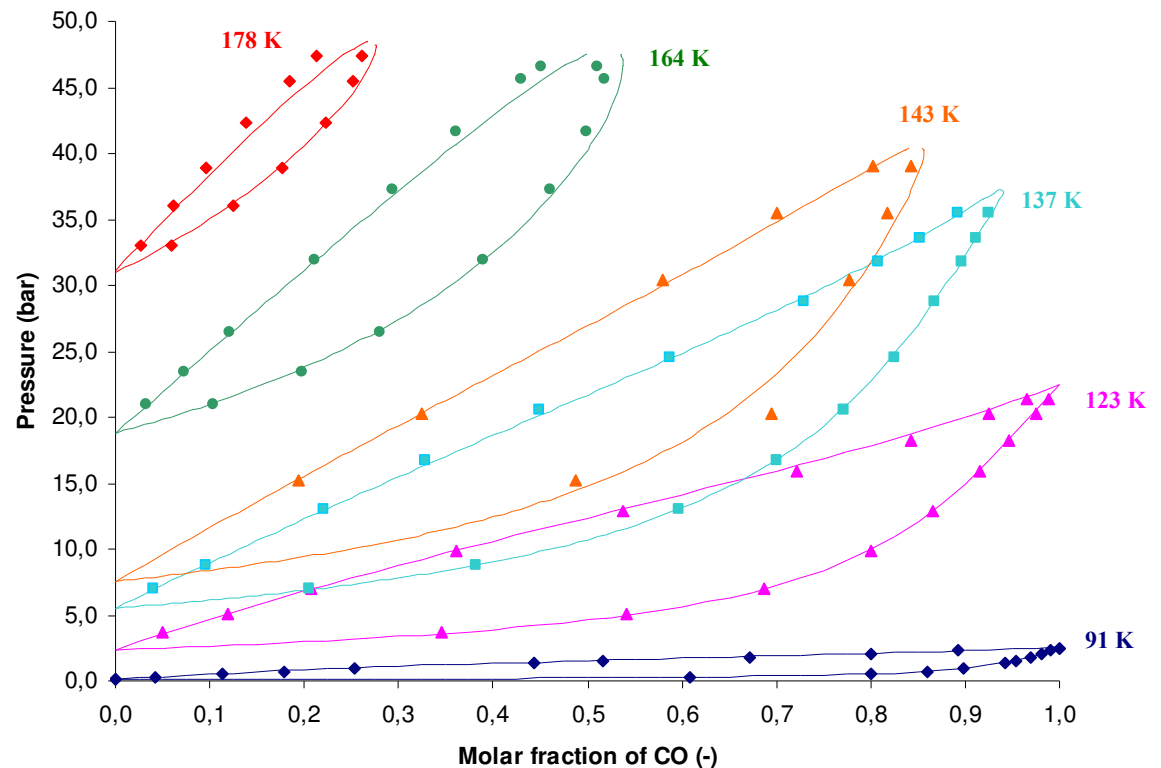
Property package development methodology

■ Property package development methodology



Example of development

- Development of a property package dedicated to Carbon Monoxide separation-purification unit simulation
 - Mixture content : N₂, CO, CH₄, Ar, H₂
 - Validity range : 1-50 bar 90-150 K
 - Peng-Robinson equation of state, conventional mixing rules
 - Calibration of binary interaction coefficient (for each binary of the system) on experimental data coming from literature (T, p, x, y)
 - Ex: CO-CH₄



Conclusions and future steps



- Appropriation and implementation of the “Thermodynamic Property Package” concept
 - Not yet a common practice but it will be in a near future
- Final tests to be done in Belsim-Vali environment
- Feasibility tests to adapt in-house simulation models (process modelling component) to CAPE-OPEN unit operation standards



Thank you for your attention

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