ProSim

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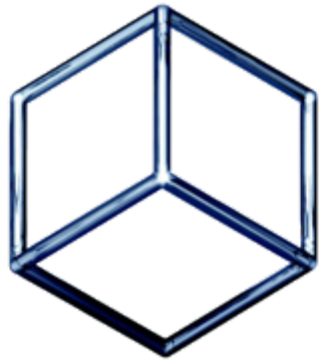

SimuLis

CO-LaN

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# CAPE-OPEN and Simulis® Thermodynamics enable you to use rigorous thermodynamics in MATLAB®

# Contents

- CAPE-OPEN / CO-LaN
- ProSim
- What is Simulis®?
- Simulis® Thermodynamics
- CAPE-OPEN and Simulis® Thermodynamics
- MATLAB® toolbox
- MATLAB® example
- Conclusions and perspectives

- A freely available industry standard for interfaces between software components making up process simulation tools
- The success of a collaboration between software vendors, end-users and academics
- A proven technology implemented in most process simulation tools
- A growing adhesion by process simulation market leaders
- CO-LaN: a group of end users taking responsibility for putting resources together to support ongoing work on the standard

ProSim

- **Skills and competences**
  - Process modeling, simulation and optimization
  - Thermodynamic calculations
  - Kinetic parameters fitting
  - Equipment sizing and design
  - Energy integration and optimization
  - Process data management

# What is Simulis®?

## Generic name given to the new software component suite of ProSim

- **New architecture**
  - Component-oriented approach applied to
    - Pure substance properties
    - Thermodynamic calculations
    - Chemical reactions
    - Unit operations
  - Easily integrated within a client application (COM)
    - Visual C++, Visual Basic, Delphi, C#, … even Visual FORTRAN
- **Based on validated code and useful services**
  - Wrapping of existing codes
    - Efficiency
    - Reliability
    - Ease-of-use

# What is Simulis®?

## Generic name given to the new software component suite of ProSim

- **Offering useful services**
  - Related services
    - Unit conversions
    - Experimental data fitting and estimation
    - Pseudo components property generation
    - Data analysis
- **Commercially available components**
  - Simulis® Conversions
    - Quantities and unit conversions management
  - Simulis® Properties
    - Pure substances properties (constant or temperature dependent) server
  - Simulis® Thermodynamics
    - Thermodynamic properties and equilibrium calculation server

# Simulis® Thermodynamics

## Thermodynamic properties and phase equilibrium calculation server for pure substances and mixtures (up to 200 compounds).

- **Properties and derivatives**
  - Transport properties (Cp, Cv, μ, λ, …)
  - Thermodynamic properties (H, S, U, …)
  - Compressibility properties (Z, Cp/Cv, …)
  - Non-ideal properties (γ, Φ, Ln(Φ), …)
  - Pseudo critical properties (Tc, Pc, Vc, Zc)
- **Equilibrium**
  - Liquid-Vapor (TP, HP, SP, ωT, ωP, UV, …)
  - Liquid-Liquid (TP)
  - Liquid-Liquid-Vapor (TP, HP, ωP)
  - Liquid-Vapor phase envelope
  - Liquid-Vapor equilibrium constants
  - Liquid-Liquid equilibrium constants
- **Thermodynamic models**
  - Soave-Redlich-Kwong (SRK)
  - Peng-Robinson (PR)
  - Lee-Kessler-Plöcker (LKP)
  - Benedict-Webb-Rubin modified Starling (BWRS)
  - Ideal
  - Wilson
  - NRTL
  - Margules
  - UNIFAC (original, Dortmund, Larsen, PSRK, LL)
  - UNIQUAC
  - Engels
  - Chao-Seader
  - Sour Water
  - Amines and acid gases
  - MHV2
  - ULPDHS …

**Simulis® Thermodynamics is provided with a pure compound database containing over 1700 pure substances.**

ProSim

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## CAPE-OPEN Thermo « plug »:

- Successfully tested with:
  - Aspen Plus (AspenTech)
  - Aspen Hysys (AspenTech)
  - PRO/II (SimSci)
  - gPROMS (PSE)
  - Xist (HTRI)
- Tests in progress with:
  - INDISS (RSI)
  - VALI (Belsim)

## CAPE-OPEN Thermo « socket »:

- Successfully tested with:
  - Aspen Properties
  - MultiFlash (Infochem)
  - PPDS (TUV NEL)

# MATLAB® toolbox

- **Over 550 MATLAB® functions allow:**
  - to calculate thermodynamic properties
  - to calculate phase equilibrium
  - to edit data with standard dialogs
  - to load and save data with standard functions
  - to create, deploy and use Simulis® data packages
  - to define your thermodynamic models
  - to access pure substances properties
  - to access binary interaction parameters
  - to convert quantities
  - …
  - and, of course, to benefit from CAPE-OPEN compliance

**A Microsoft® Excel add-in of Simulis® Thermodynamics is also available and is provided together with a MATLAB® toolbox.**

ProSim

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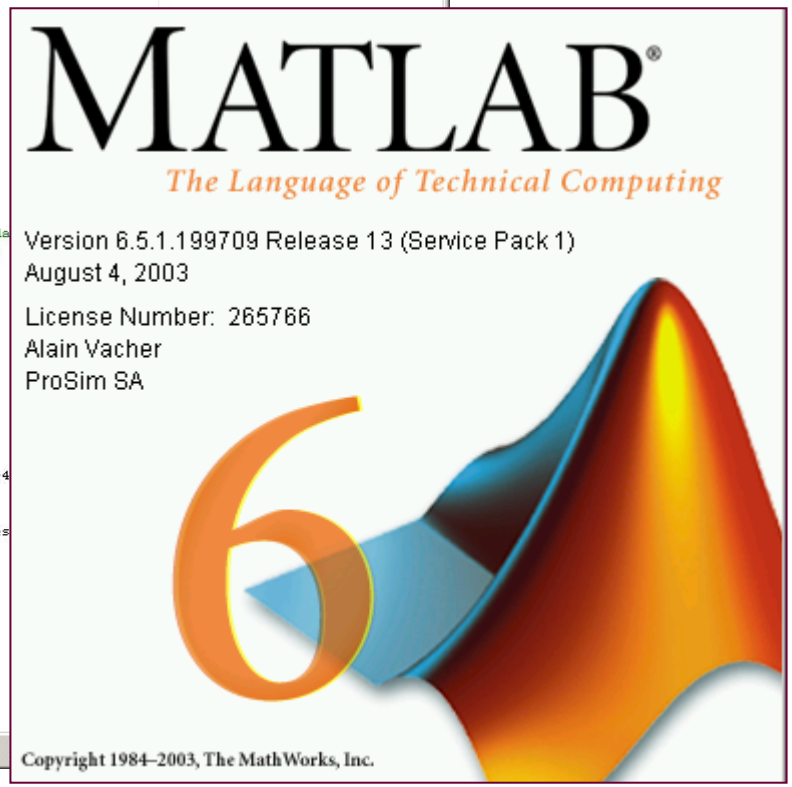
# MATLAB® example

Editor - C:\MagicBox\AIChE_Example.m

File Edit Text Cell Tools Debug Desktop Window Help

```
function [] = AIChE_Example
%
% Simulis Thermodynamics
% AIChE 2005 - Cincinnati, OH
% Michel PONS - Alain VACHER
%
% 1- Thermodynamic calculator creation
scal = stCALCreate;
% 2- Unit system edition using a standard Simulis dialog
% 2.1- Input unit system edition (atm, °C)
modified = stCALSystemEdit(scal,1);
% 2.2- Output unit system edition (J/mol/K)
modified = stCALSystemEdit(scal,2);
% 3- Thermodynamic calculator edition using another standa
%    (Hyprotech Property Package (HDA - SRK) is selected)
modified = stCALEdit(scal);
% 4- Input data
% 4.1- Composition
fractions = [0.2 0.2 0.2 0.2 0.2];
% 4.2- Composition type (0 = molar, 1 = mass)
typeFrac = 0;
% 4.3- Result type (0 = molar, 1 = mass)
typeRes = 0;
% 4.4- Pressure (atm)
pressure = 1.0;
% 4.5- Temperatures (°C)
resTemperatures = [-100.0 -90.0 -80.0 -70.0 -60.0 -50.0 -4
% 5- Vapor Cp calculations
for i=1:11,
  [ resCps(i) ] = stCALCpV( scal, resTemperatures(i), pres
end
resCps
% 6- Results plot
hpl = plot(resTemperatures,resCps,'-b');
title('-  Vapor Cp calculations  -');
xlabel('Temperature (°C)');
ylabel('Cp (J/mol/K)');
grid on;
% 7- Free thermodynamic calculator
stCALFree(scal);
```




**Use of a CAPE-OPEN Property Package created by Aspen Properties throughout the thermodynamic socket of Simulis® Thermodynamics within MATLAB®**

ProSim

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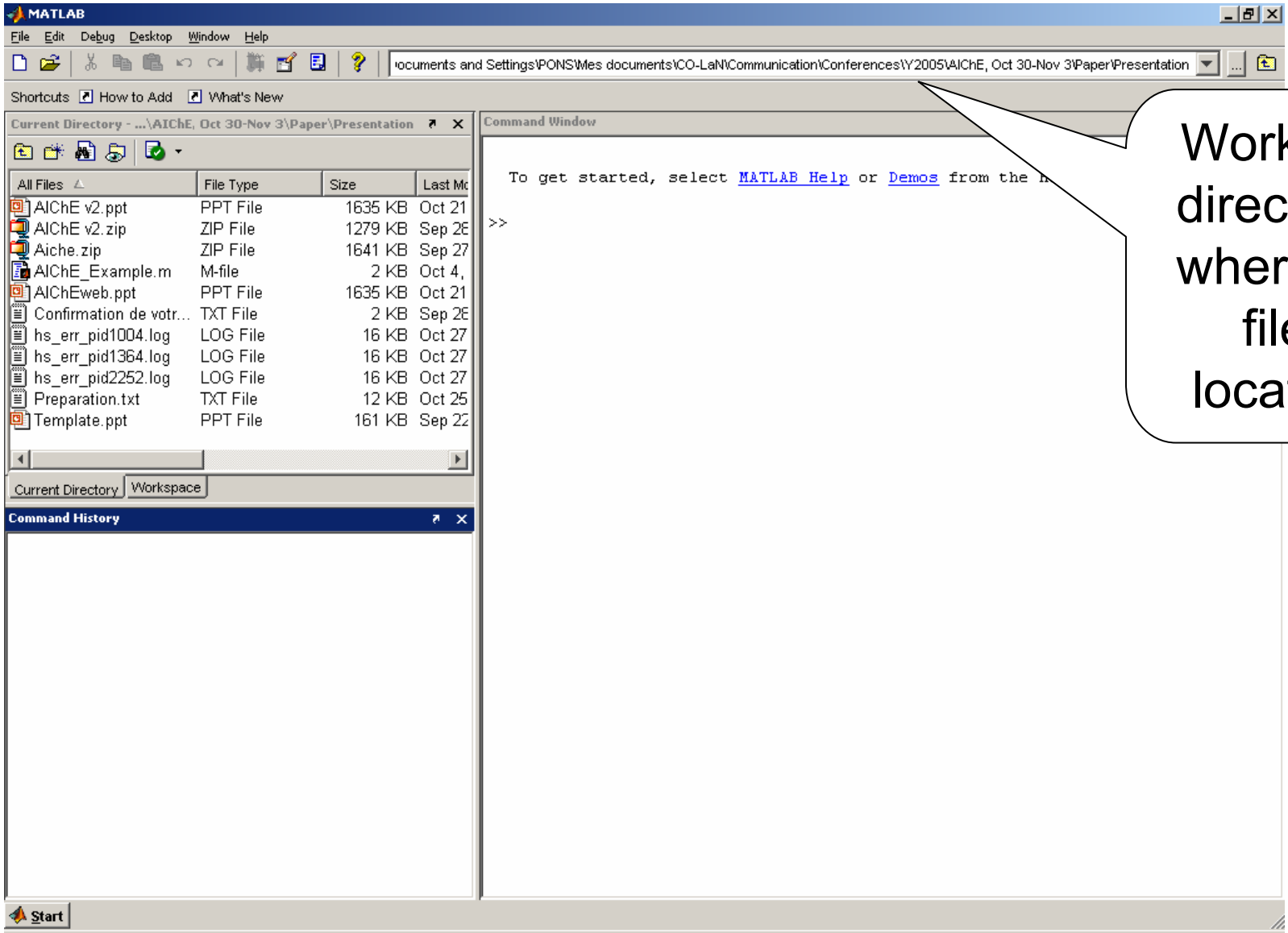
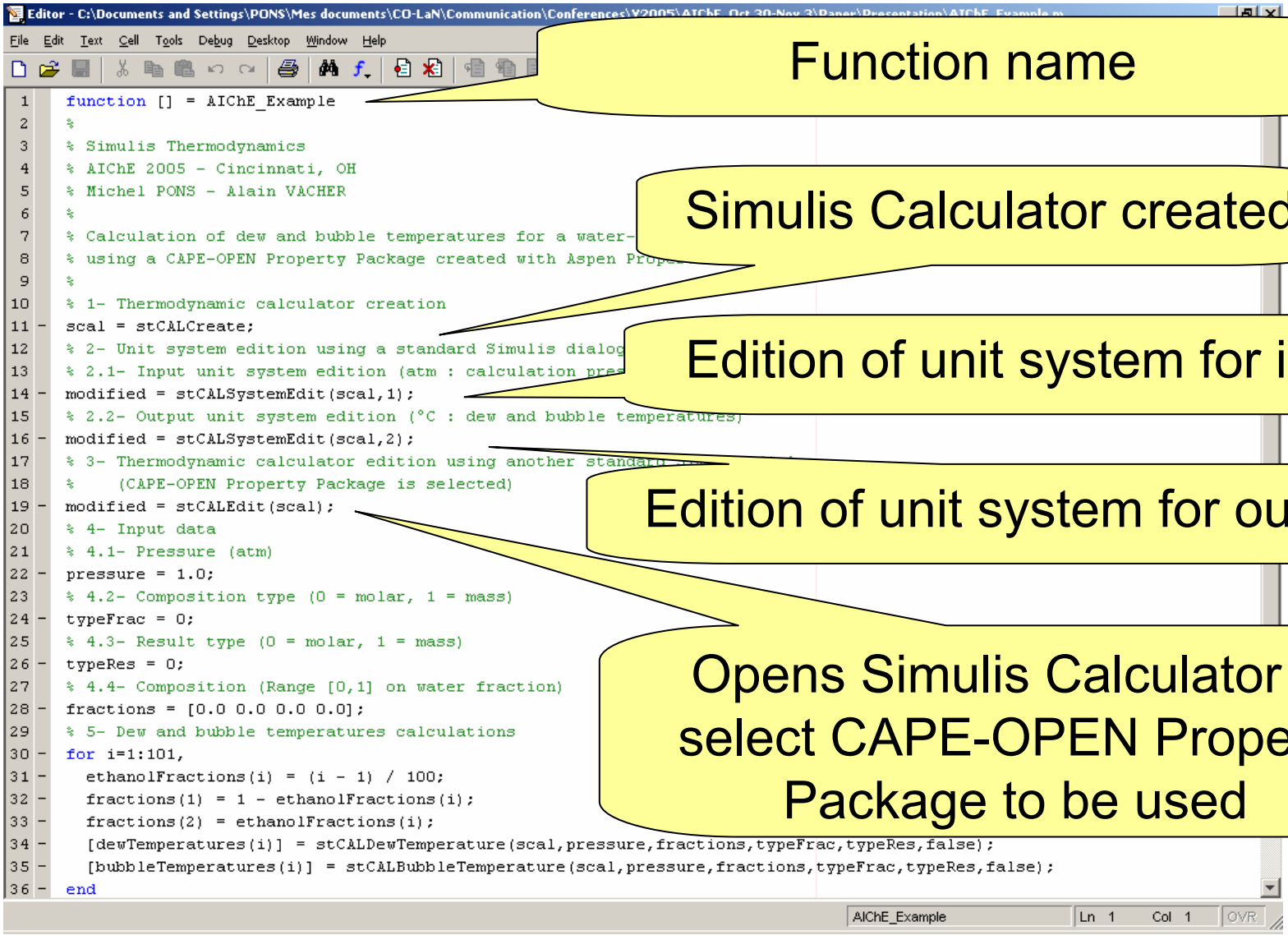
# Opening MatLab

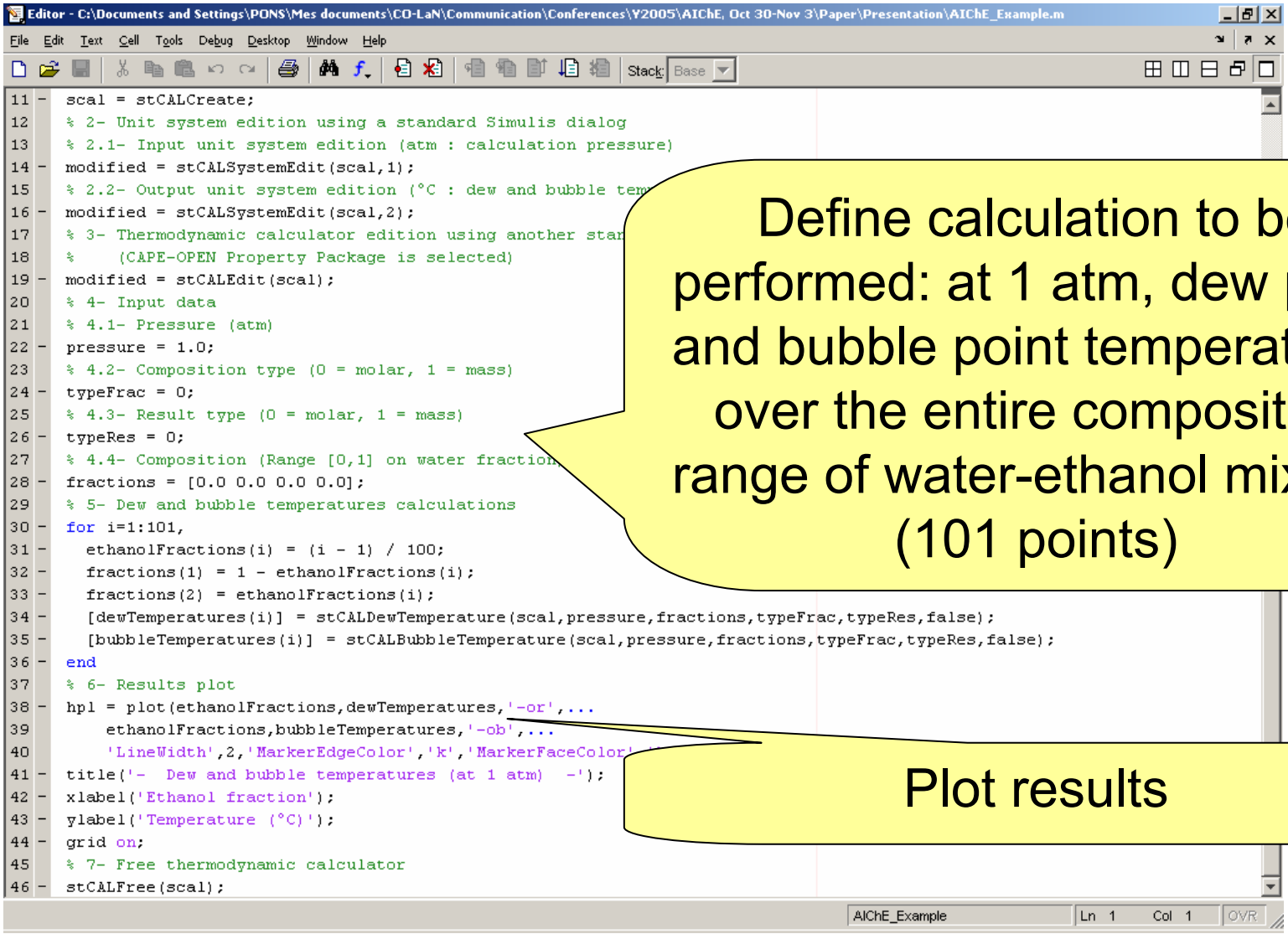



Working directory where m file located

# Editing m file



# Editing next




Define calculation to be performed: at 1 atm, dew point and bubble point temperatures over the entire composition range of water-ethanol mixture (101 points)

Plot results

ProSim

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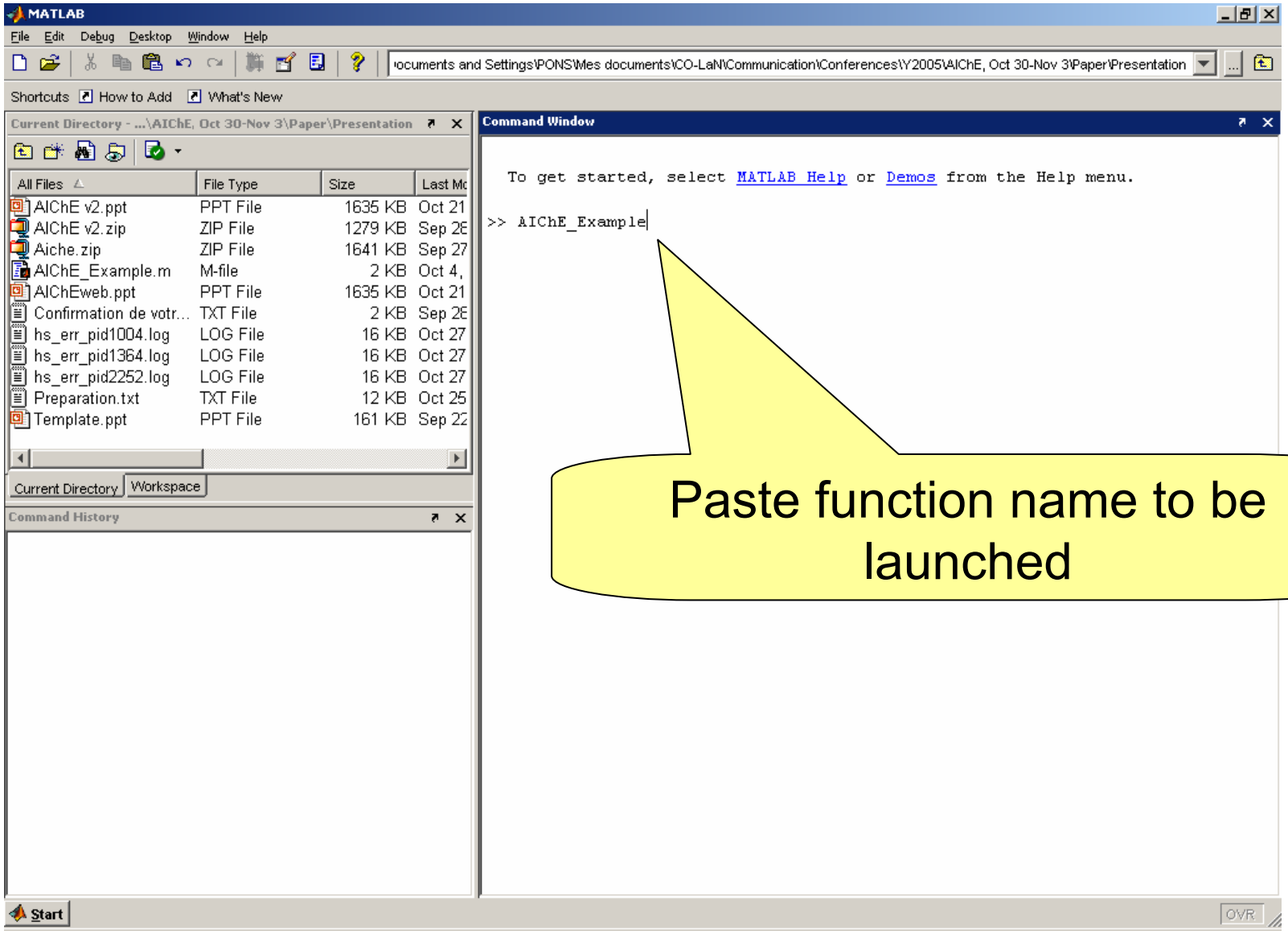
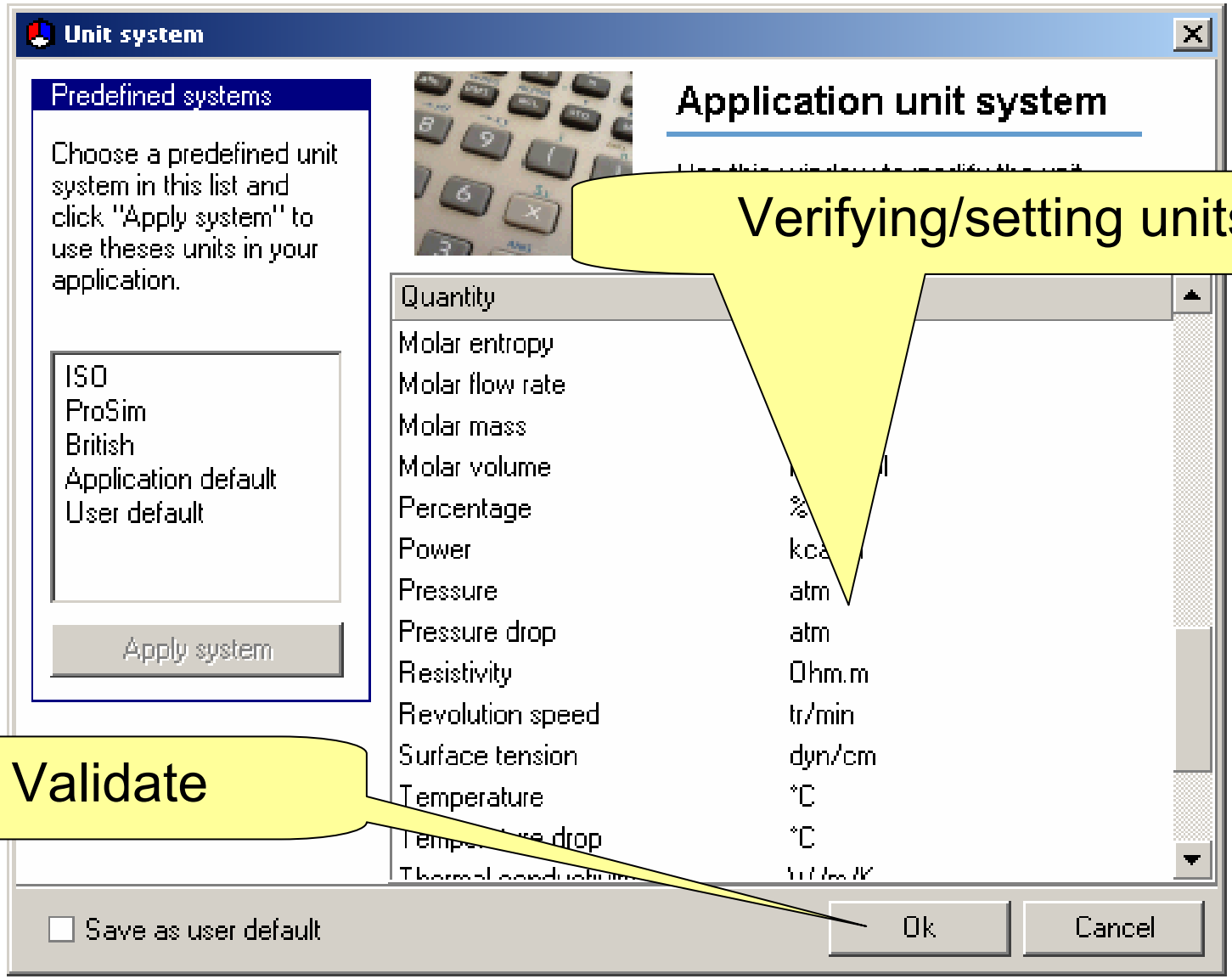
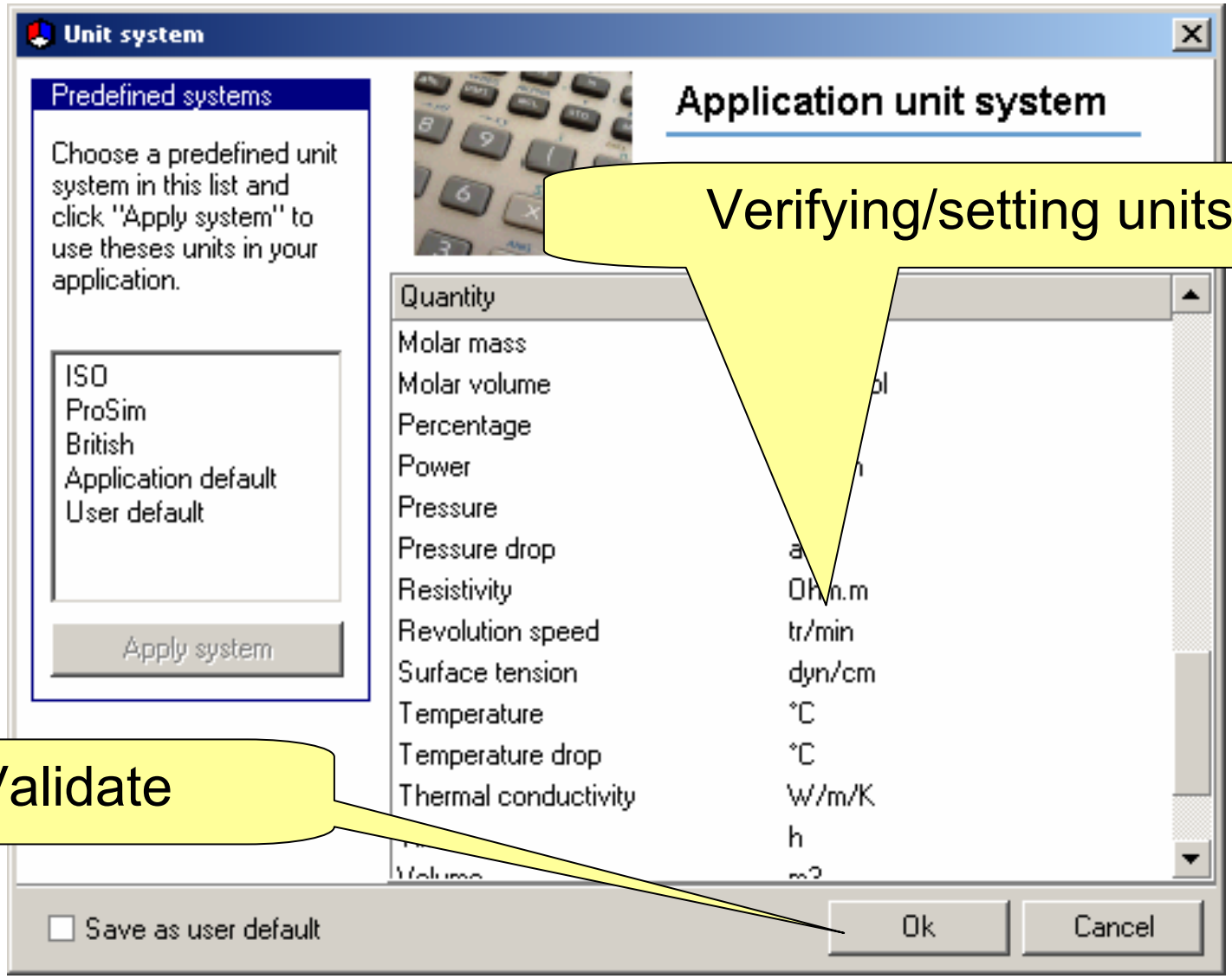
# Launching m file execution



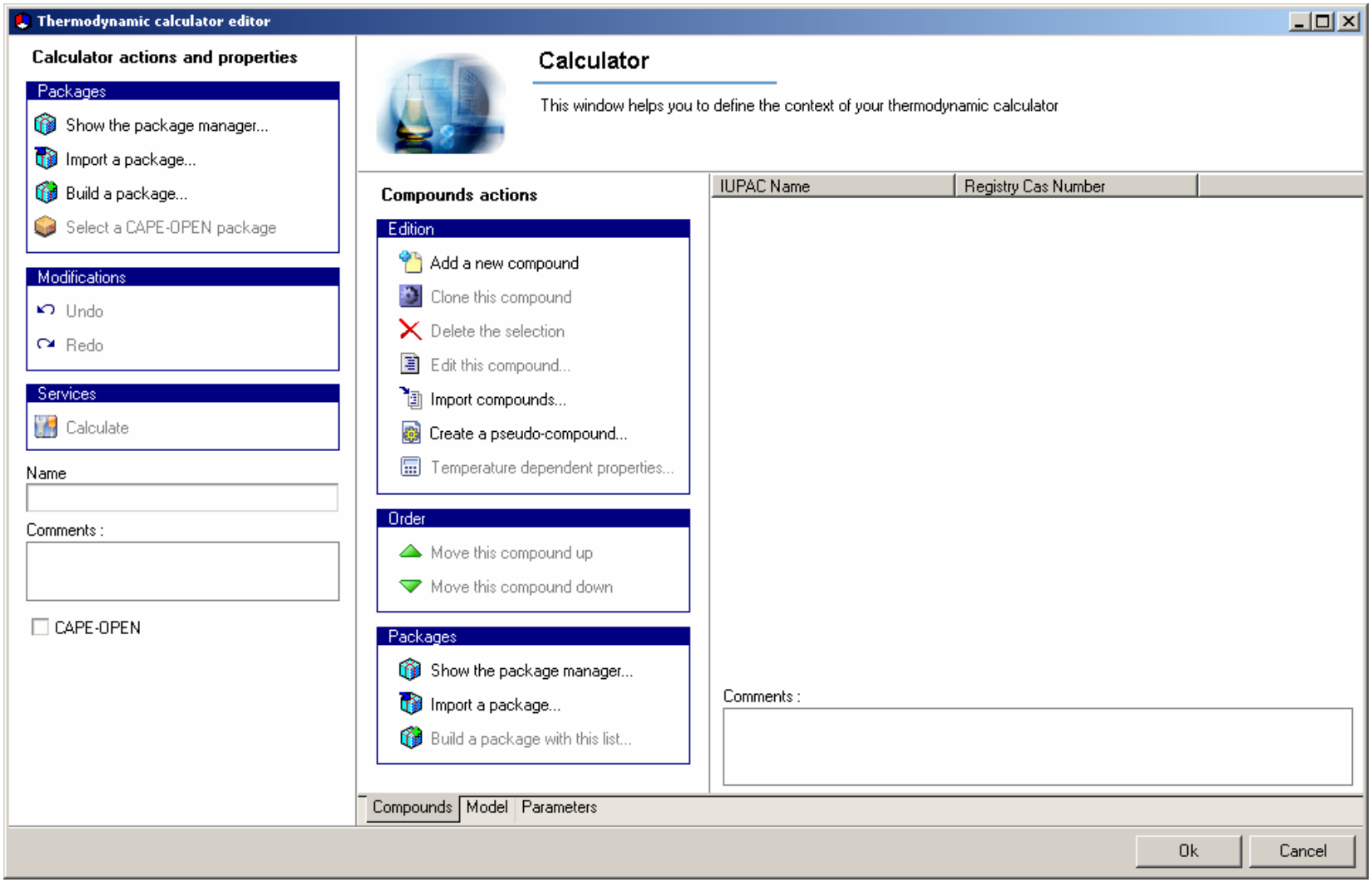
# Setting unit system for input



# Setting unit system for output



# Simulis Calculator opens

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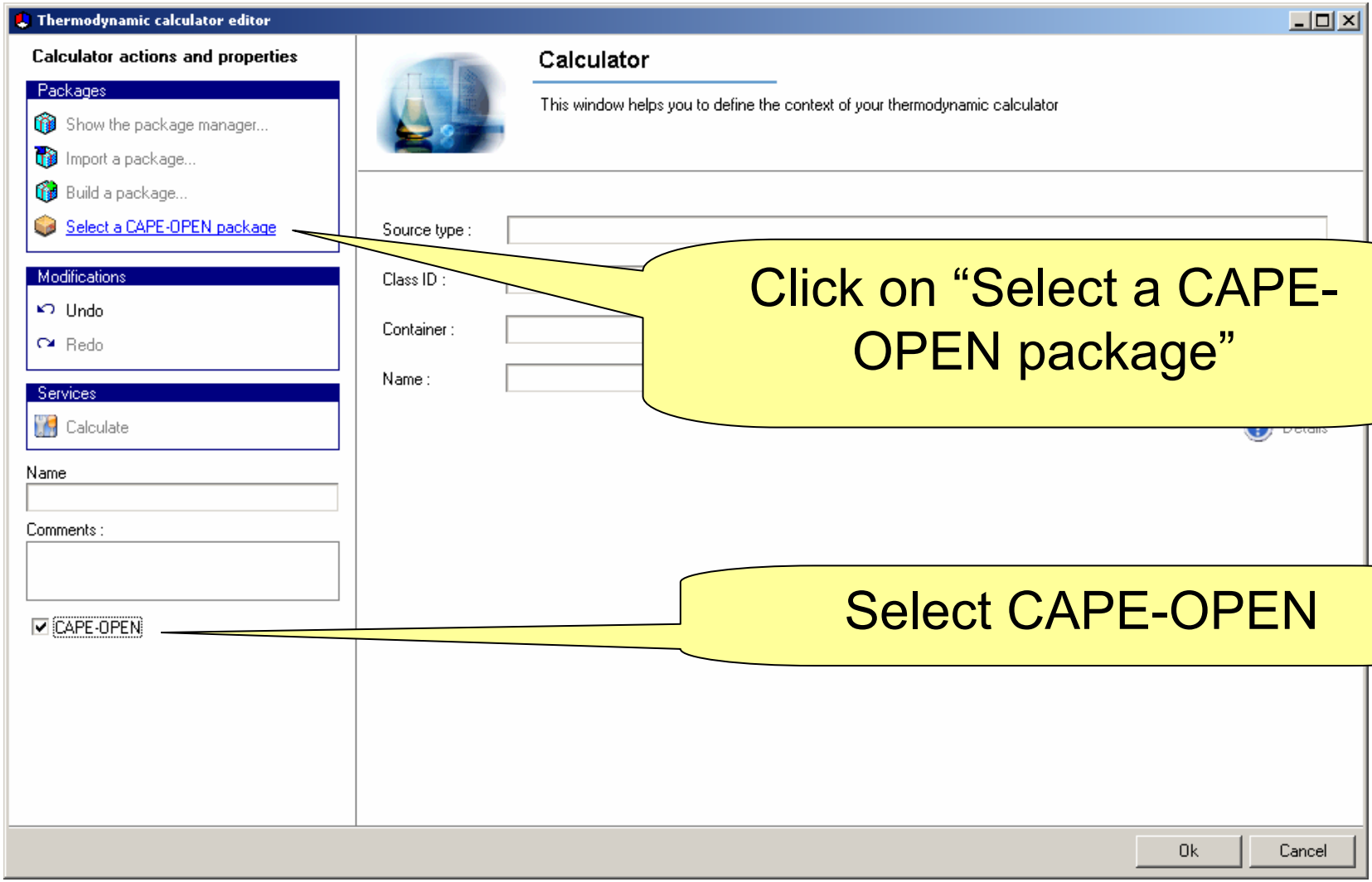
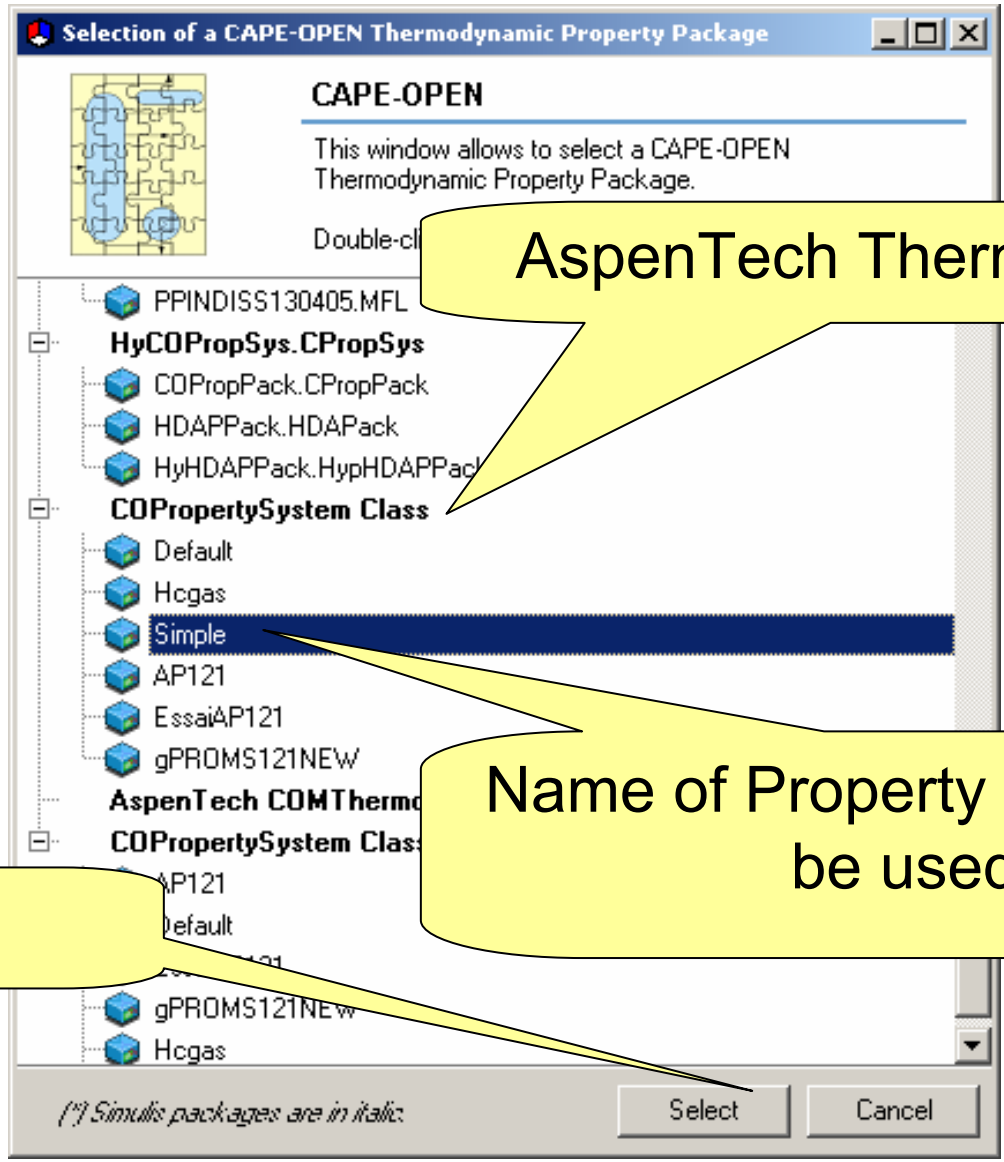
# Asking for list of available CAPE-OPEN Property Packages




Click on “Select a CAPE-OPEN package”

Select CAPE-OPEN

# List available CAPE-OPEN Property Packages and select one

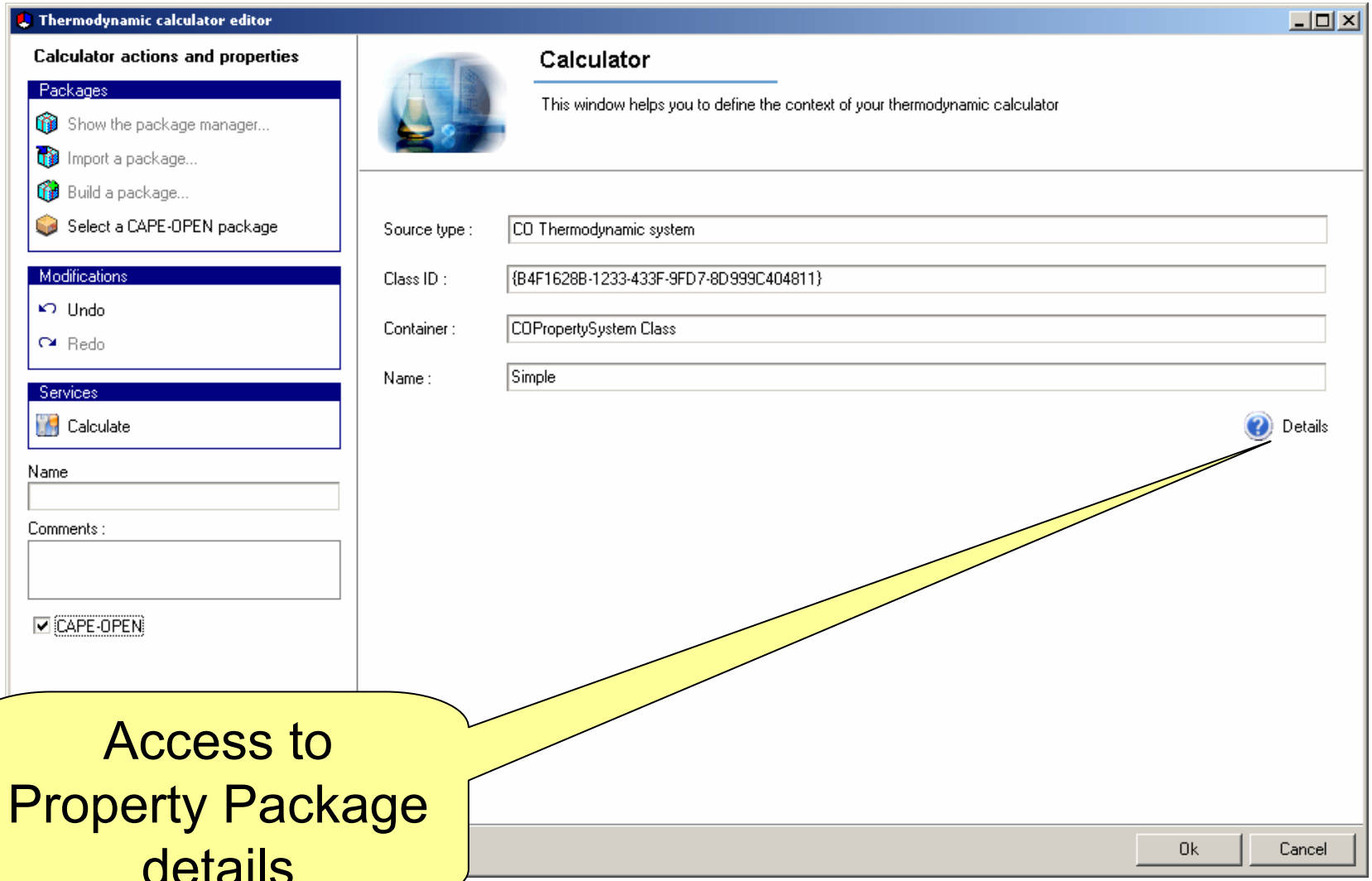



AspenTech Thermo System

Name of Property Package to be used

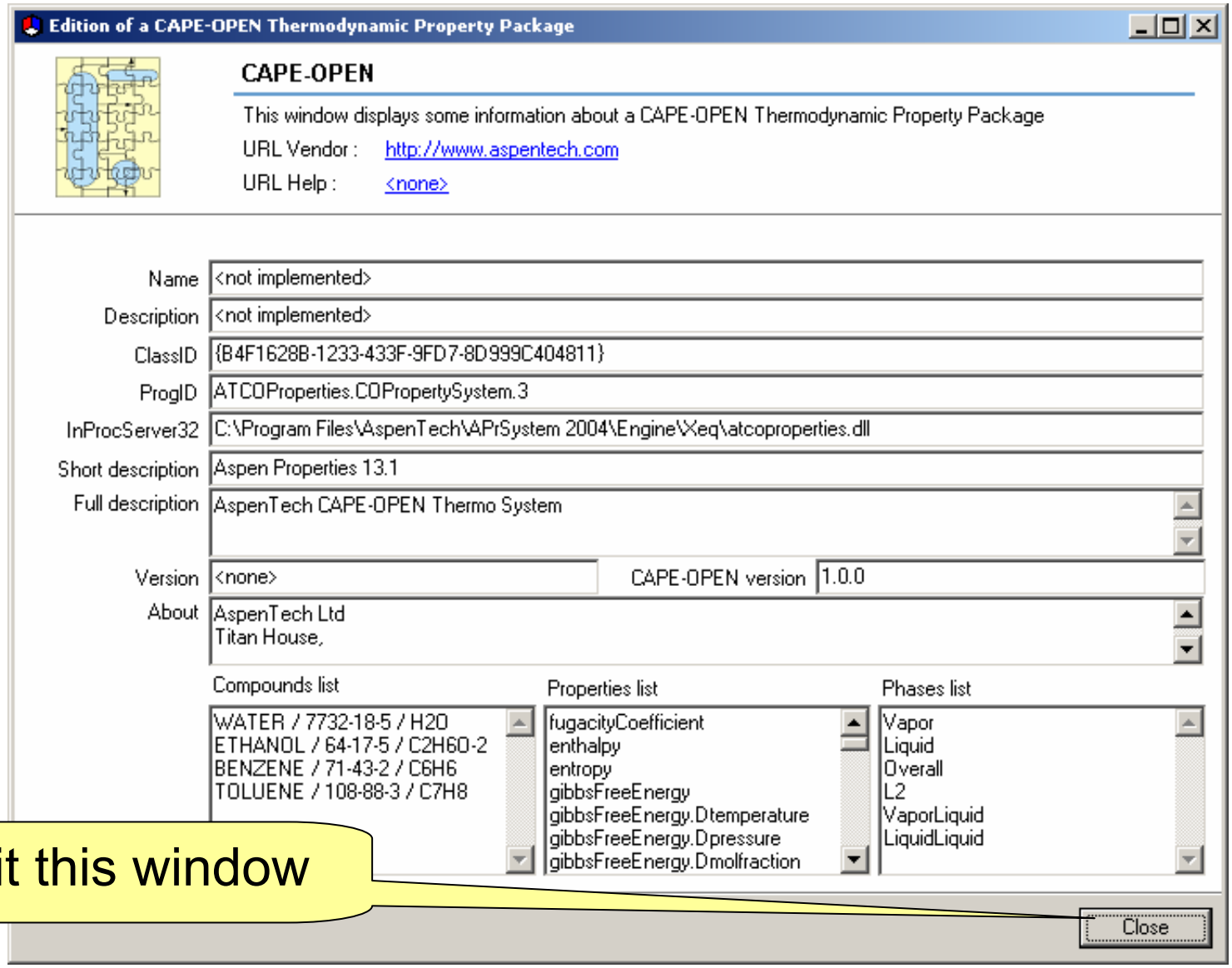
Validate

# Property Package selection performed




Access to Property Package details

# AspenTech Property Package displayed




Exit this window

ProSim

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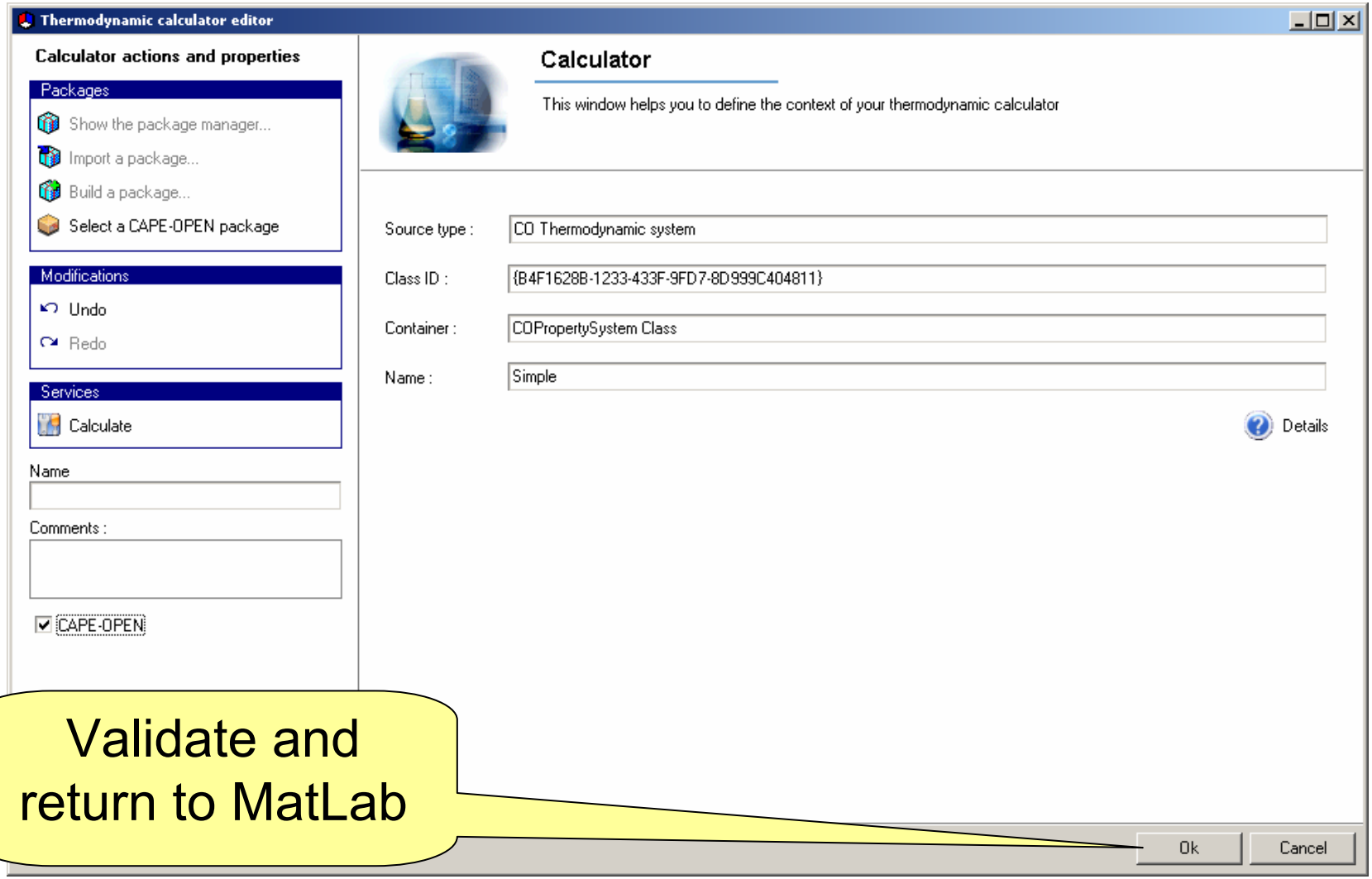
# Property Package selected




Validate and return to MatLab

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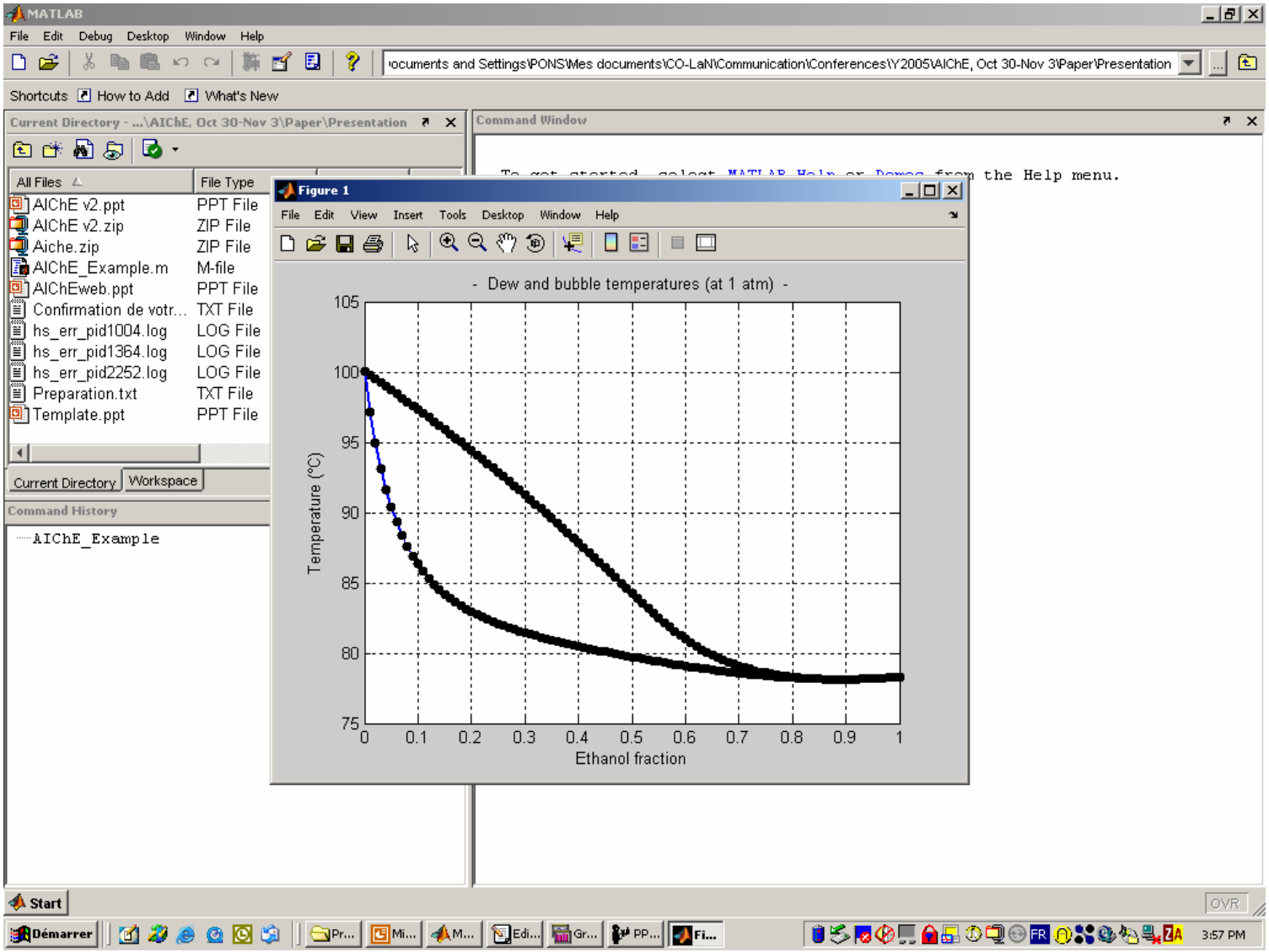
# Results displayed



# Component based environments:

- Software interoperability
  - Fundamental architecture choice
- Software interchangeability
  - CAPE-OPEN standard
- Quality improvement of studies run
  - Choice of the best component for a given case
- Reduction of development time (costs)
  - A judicious assembly
- Best productivity for
  - End-users..
  - … and developers

# Cheaper, better and faster design, operation and control of processes

- **Plug-and-play**
  - Ability to seamlessly integrate a component from the library of foreign objects (unit operations, thermo models, solvers etc.).
  - Ability to seamlessly integrate in-house proprietary components in commercial environments.
- **Niche software**
  - Ability to link specific niche modules to the simulators. Small and niche software vendors will provide CO-compliant components.
- **Return On Investment**
  - Individual studies will cost less because of the technical advantages of being able to mix-and-match.
  - Plug-and-play capacity will stimulate the market and create new opportunities.