



ProSim

Alain VACHER
Stratège Bâtiment A
BP 2738
F-31312 LABEGE Cedex
FRANCE
www.prosim.net



SimuLis

**CAPE-OPEN and Simulis[®] Thermodynamics
enable you to use rigorous thermodynamics in
MATLAB[®]**



CO²LaN

Dr Michel PONS
CAPE-OPEN Laboratories Network
32 rue Raulin
F-69007 LYON
FRANCE
www.colan.org

- ▼ **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**





Skills and competences

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

PHARMACIA

NOVARTIS

ORION

SINTEF

ARKEMA

Gaz de France

Schering-Plough

L'ORÉAL

DISLAUB
Les Distilleries de l'Aube

Technip

Ciba

cea

AstraZeneca
INTERNATIONAL

AIR LIQUIDE

CNES

ORICA



IFP

sanofi aventis
L'essentiel c'est la santé.

TOTAL

Rhodia

CO₂LaN



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



Thermodynamic properties and phase equilibrium calculation server for pure substances and mixtures (up to 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
- 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.



▼ 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)**



▼ 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

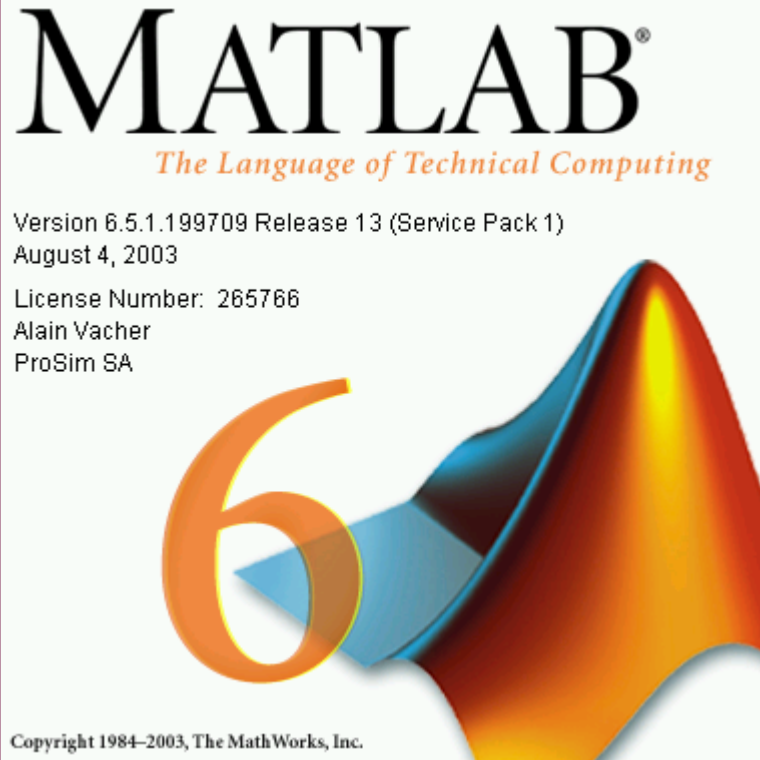
A Microsoft® Excel add-in of Simulis® Thermodynamics is also available and is provided together with a MATLAB® toolbox.



MATLAB® example

```
Editor - C:\MagicBox\AICHe_Example.m
File Edit Text Cell Tools Debug Desktop Window Help
Stack: Ba...

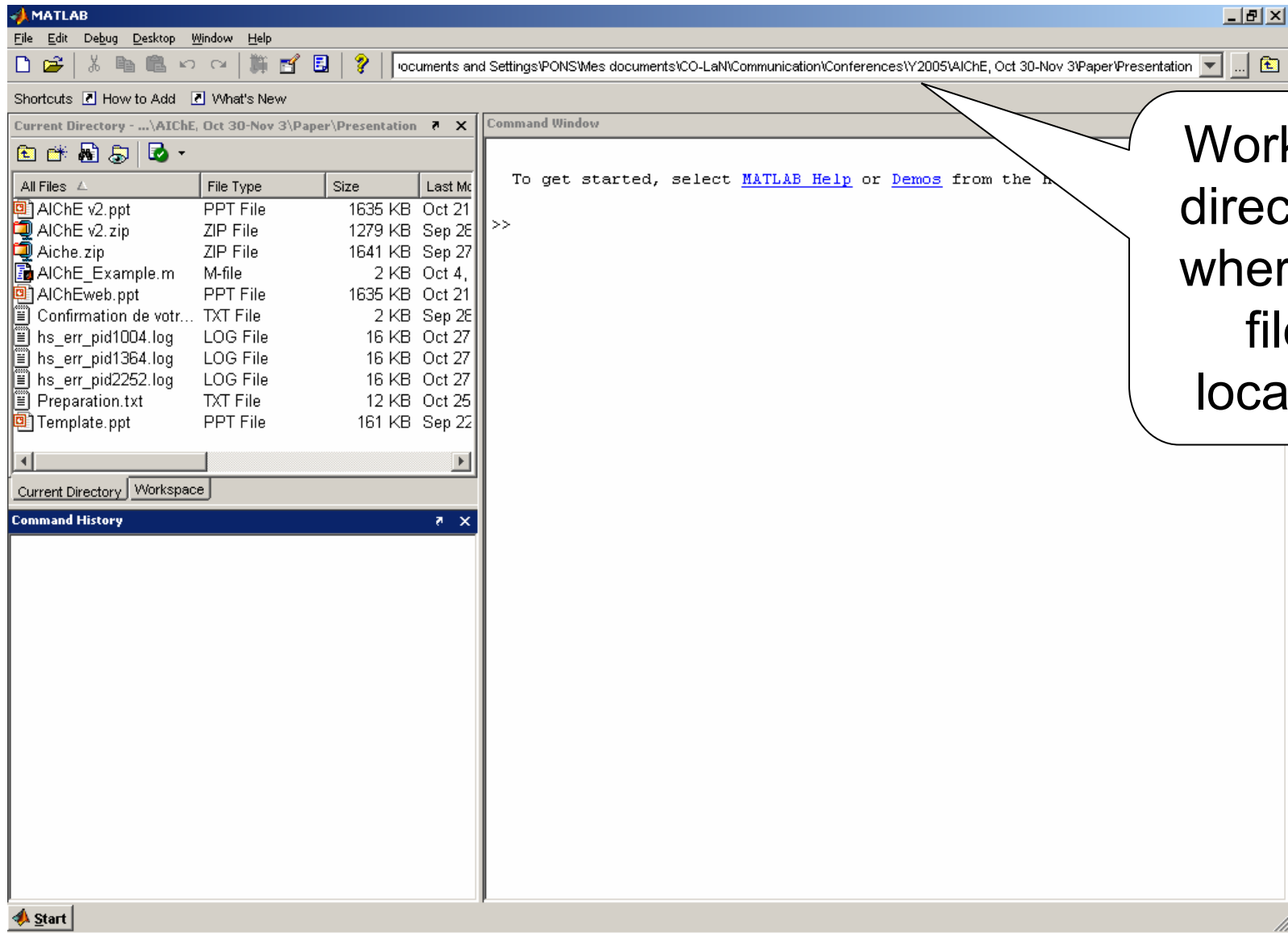
1 function [] = AICHe_Example
2 %
3 % Simulis Thermodynamics
4 % AICHe 2005 - Cincinnati, OH
5 % Michel PONS - Alain VACHER
6 %
7 % 1- Thermodynamic calculator creation
8 scal = stCALCreate;
9 % 2- Unit system edition using a standard Simulis dialog
10 % 2.1- Input unit system edition (atm, °C)
11 modified = stCALSystemEdit(scal,1);
12 % 2.2- Output unit system edition (J/mol/K)
13 modified = stCALSystemEdit(scal,2);
14 % 3- Thermodynamic calculator edition using another standa
15 % (Hyprotech Property Package (HDA - SRK) is selected)
16 modified = stCALEdit(scal);
17 % 4- Input data
18 % 4.1- Composition
19 fractions = [0.2 0.2 0.2 0.2 0.2];
20 % 4.2- Composition type (0 = molar, 1 = mass)
21 typeFrac = 0;
22 % 4.3- Result type (0 = molar, 1 = mass)
23 typeRes = 0;
24 % 4.4- Pressure (atm)
25 pressure = 1.0;
26 % 4.5- Temperatures (°C)
27 resTemperatures = [-100.0 -90.0 -80.0 -70.0 -60.0 -50.0 -4
28 % 5- Vapor Cp calculations
29 for i=1:11,
30     [ resCps(i) ] = stCALCpV( scal, resTemperatures(i), pres
31 end
32 resCps
33 % 6- Results plot
34 hpl = plot(resTemperatures,resCps,'-b');
35 title('- Vapor Cp calculations -');
36 xlabel('Temperature (°C)');
37 ylabel('Cp (J/mol/K)');
38 grid on;
39 % 7- Free thermodynamic calculator
40 stCALFree(scal);
```



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



Opening MatLab



Working directory where m file located



Editing m file

```
Editor - C:\Documents and Settings\PONS\Mes documents\CO-LaN\Communication\Conferences\Y2005\AICHE_Oct 30-Nov 3\Paper\Prerentation\AICHE_Example.m
File Edit Text Cell Tools Debug Desktop Window Help
1 function [] = AICHe_Example
2 %
3 % Simulis Thermodynamics
4 % AICHE 2005 - Cincinnati, OH
5 % Michel PONS - Alain VACHER
6 %
7 % Calculation of dew and bubble temperatures for a water-
8 % using a CAPE-OPEN Property Package created with Aspen Prop
9 %
10 %
11 % 1- Thermodynamic calculator creation
12 scal = stCALCreate;
13 % 2- Unit system edition using a standard Simulis dialog
14 % 2.1- Input unit system edition (atm : calculation pres
15 modified = stCALSystemEdit(scal,1);
16 % 2.2- Output unit system edition (°C : dew and bubble temperatures)
17 modified = stCALSystemEdit(scal,2);
18 % 3- Thermodynamic calculator edition using another standard
19 % (CAPE-OPEN Property Package is selected)
20 modified = stCALEdit(scal);
21 % 4- Input data
22 % 4.1- Pressure (atm)
23 pressure = 1.0;
24 % 4.2- Composition type (0 = molar, 1 = mass)
25 typeFrac = 0;
26 % 4.3- Result type (0 = molar, 1 = mass)
27 typeRes = 0;
28 % 4.4- Composition (Range [0,1] on water fraction)
29 fractions = [0.0 0.0 0.0 0.0];
30 % 5- Dew and bubble temperatures calculations
31 for i=1:101,
32 ethanolFractions(i) = (i - 1) / 100;
33 fractions(1) = 1 - ethanolFractions(i);
34 fractions(2) = ethanolFractions(i);
35 [dewTemperatures(i)] = stCALDewTemperature(scal,pressure,fractions,typeFrac,typeRes,false);
36 [bubbleTemperatures(i)] = stCAlBubbleTemperature(scal,pressure,fractions,typeFrac,typeRes,false);
37 end
```

Function name

Simulis Calculator created

Edition of unit system for input

Edition of unit system for output

Opens Simulis Calculator to select CAPE-OPEN Property Package to be used



Editing next

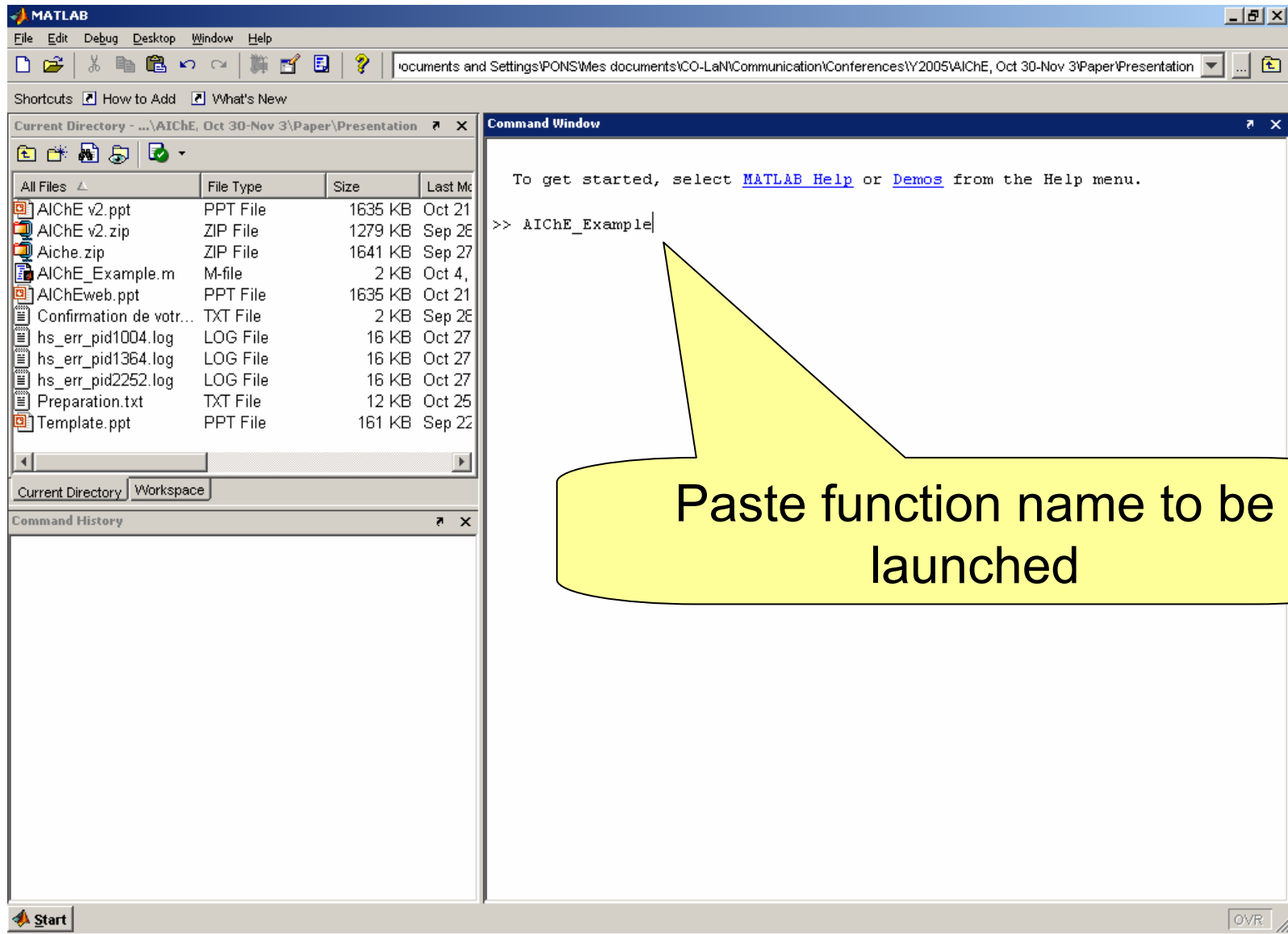
```
Editor - C:\Documents and Settings\PONS\Mes documents\CO-LaN\Communication\Conferences\Y2005\AICHe, Oct 30-Nov 3\Paper\Presentation\AICHe_Example.m
File Edit Text Cell Tools Debug Desktop Window Help
Stack: Base
11 scal = stCALCreate;
12 % 2- Unit system edition using a standard Simulis dialog
13 % 2.1- Input unit system edition (atm : calculation pressure)
14 modified = stCALSystemEdit(scal,1);
15 % 2.2- Output unit system edition (°C : dew and bubble temp
16 modified = stCALSystemEdit(scal,2);
17 % 3- Thermodynamic calculator edition using another stan
18 % (CAPE-OPEN Property Package is selected)
19 modified = stCALEdit(scal);
20 % 4- Input data
21 % 4.1- Pressure (atm)
22 pressure = 1.0;
23 % 4.2- Composition type (0 = molar, 1 = mass)
24 typeFrac = 0;
25 % 4.3- Result type (0 = molar, 1 = mass)
26 typeRes = 0;
27 % 4.4- Composition [Range [0,1] on water fraction]
28 fractions = [0.0 0.0 0.0 0.0];
29 % 5- Dew and bubble temperatures calculations
30 for i=1:101,
31 ethanolFractions(i) = (i - 1) / 100;
32 fractions(1) = 1 - ethanolFractions(i);
33 fractions(2) = ethanolFractions(i);
34 [dewTemperatures(i)] = stCALDewTemperature(scal,pressure,fractions,typeFrac,typeRes,false);
35 [bubbleTemperatures(i)] = stCAlBubbleTemperature(scal,pressure,fractions,typeFrac,typeRes,false);
36 end
37 % 6- Results plot
38 hpl = plot(ethanolFractions,dewTemperatures,'-or',...
39 ethanolFractions,bubbleTemperatures,'-ob',...
40 'LineWidth',2,'MarkerEdgeColor','k','MarkerFaceColor','r');
41 title('- Dew and bubble temperatures (at 1 atm) -');
42 xlabel('Ethanol fraction');
43 ylabel('Temperature (°C)');
44 grid on;
45 % 7- Free thermodynamic calculator
46 stCALFree(scal);
```

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



Launching m file execution



The image shows a screenshot of the MATLAB software interface. The main window displays a file explorer on the left and a Command Window on the right. The file explorer shows a list of files in the current directory, including 'AICHe_Example.m'. The Command Window shows the command '>> AICHe_Example' entered. A yellow callout box points to the command with the text 'Paste function name to be launched'.

Current Directory - ...\AICHe, Oct 30-Nov 3\Paper\Presentation

All Files	File Type	Size	Last Modified
AICHe v2.ppt	PPT File	1635 KB	Oct 21
AICHe v2.zip	ZIP File	1279 KB	Sep 26
Aiche.zip	ZIP File	1641 KB	Sep 27
AICHe_Example.m	M-file	2 KB	Oct 4,
AICHeWeb.ppt	PPT File	1635 KB	Oct 21
Confirmation de votr...	TXT File	2 KB	Sep 26
hs_err_pid1004.log	LOG File	16 KB	Oct 27
hs_err_pid1364.log	LOG File	16 KB	Oct 27
hs_err_pid2252.log	LOG File	16 KB	Oct 27
Preparation.txt	TXT File	12 KB	Oct 25
Template.ppt	PPT File	161 KB	Sep 22

Command Window

```
To get started, select MATLAB Help or Demos from the Help menu.  
>> AICHe_Example|
```

Paste function name to be launched



Setting unit system for input

Unit system

Predefined systems

Choose a predefined unit system in this list and click "Apply system" to use these units in your application.

- ISO
- ProSim
- British
- Application default
- User default

Apply system

Application unit system

Use this window to modify the unit

Quantity	Unit
Molar entropy	J/mol.K
Molar flow rate	mol/h
Molar mass	g/mol
Molar volume	m ³ /mol
Percentage	%
Power	kcal/h
Pressure	atm
Pressure drop	atm
Resistivity	Ohm.m
Revolution speed	tr/min
Surface tension	dyn/cm
Temperature	°C
Temperature drop	°C
Thermal conductivity	W/m.K

Save as user default

Ok Cancel

Validate

Verifying/setting units



Setting unit system for output

Unit system

Predefined systems

Choose a predefined unit system in this list and click "Apply system" to use these units in your application.

- ISO
- ProSim
- British
- Application default
- User default

Apply system

Application unit system

Quantity	Unit
Molar mass	g/mol
Molar volume	l/mol
Percentage	%
Power	W
Pressure	Pa
Pressure drop	Pa
Resistivity	Ohm.m
Revolution speed	tr/min
Surface tension	dyn/cm
Temperature	°C
Temperature drop	°C
Thermal conductivity	W/m/K
Volume	m ³

Save as user default

Ok Cancel

Validate

Verifying/setting units



Simulis Calculator opens

Thermodynamic calculator editor

Calculator actions and properties

Packages

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

Modifications

- Undo
- Redo

Services

- Calculate

Name:

Comments:

CAPE-OPEN

Calculator

This window helps you to define the context of your thermodynamic calculator

Compounds actions

Edition

- Add a new compound
- Clone this compound
- Delete the selection
- Edit this compound...
- Import compounds...
- Create a pseudo-compound...
- Temperature dependent properties...

Order

- Move this compound up
- Move this compound down

Packages

- Show the package manager...
- Import a package...
- Build a package with this list...

IUPAC Name	Registry Cas Number
------------	---------------------

Comments:

Compounds | Model | Parameters

Ok Cancel

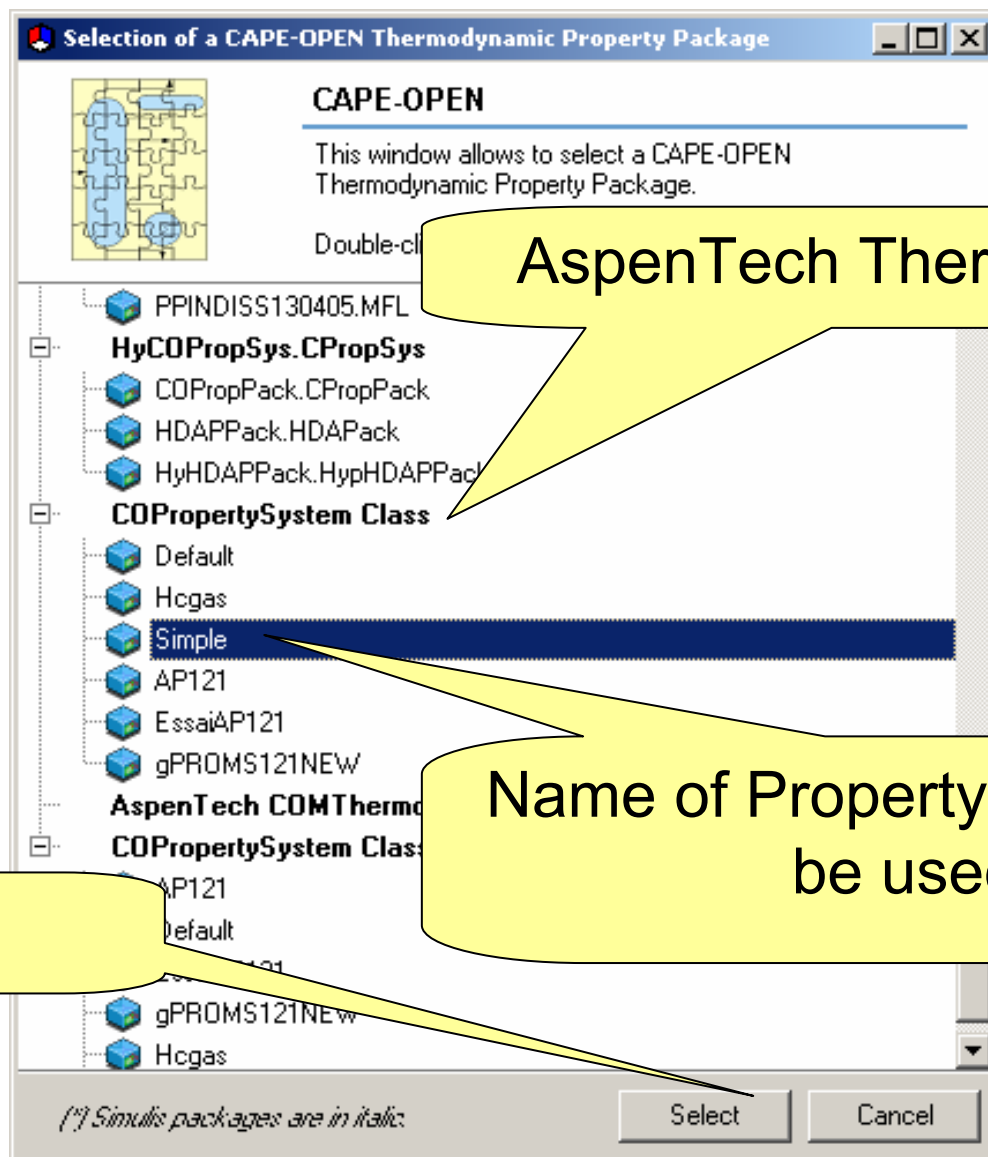


Asking for list of available CAPE-OPEN Property Packages

The screenshot shows the 'Thermodynamic calculator editor' window. On the left, under 'Calculator actions and properties', the 'Packages' section contains a list of actions: 'Show the package manager...', 'Import a package...', 'Build a package...', and 'Select a CAPE-OPEN package'. A yellow callout bubble points to the 'Select a CAPE-OPEN package' option with the text 'Click on "Select a CAPE-OPEN package"'. Below this, the 'Modifications' section has 'Undo' and 'Redo' buttons, and the 'Services' section has a 'Calculate' button. At the bottom left, there is a 'Name' field, a 'Comments' text area, and a checked checkbox labeled 'CAPE-OPEN'. A second yellow callout bubble points to this checkbox with the text 'Select CAPE-OPEN'. The main area of the window is titled 'Calculator' and contains a sub-header 'Calculator' with the text 'This window helps you to define the context of your thermodynamic calculator'. Below this are input fields for 'Source type:', 'Class ID:', 'Container:', and 'Name:'. At the bottom right of the window are 'Ok' and 'Cancel' buttons.



List available CAPE-OPEN Property Packages and select one



AspenTech Thermo System

Name of Property Package to be used

Validate



Property Package selection performed

Thermodynamic calculator editor

Calculator actions and properties

Packages

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

Modifications

- Undo
- Redo

Services

- Calculate

Name:

Comments:

CAPE-OPEN

Calculator

This window helps you to define the context of your thermodynamic calculator

Source type:

Class ID:

Container:

Name:

[Details](#)

Ok Cancel

Access to
Property Package
details



AspenTech Property Package displayed

Edition of a CAPE-OPEN Thermodynamic Property Package

CAPE-OPEN

This window displays some information about a CAPE-OPEN Thermodynamic Property Package

URL Vendor : <http://www.aspentech.com>

URL Help : [<none>](#)

Name <not implemented>

Description <not implemented>

ClassID {B4F1628B-1233-433F-9FD7-8D999C404811}

ProgID ATCOProperties.COPropertySystem.3

InProcServer32 C:\Program Files\AspenTech\APrSystem 2004\Engine\Xeql\atcoproperties.dll

Short description Aspen Properties 13.1

Full description AspenTech CAPE-OPEN Thermo System

Version <none> CAPE-OPEN version 1.0.0

About AspenTech Ltd
Titan House,

Compounds list	Properties list	Phases list
WATER / 7732-18-5 / H2O	fugacityCoefficient	Vapor
ETHANOL / 64-17-5 / C2H6O-2	enthalpy	Liquid
BENZENE / 71-43-2 / C6H6	entropy	Overall
TOLUENE / 108-88-3 / C7H8	gibbsFreeEnergy	L2
	gibbsFreeEnergy.Dtemperature	VaporLiquid
	gibbsFreeEnergy.Dpressure	LiquidLiquid
	gibbsFreeEnergy.Dmolfraction	

Close

Exit this window



Property Package selected

Thermodynamic calculator editor

Calculator actions and properties

Packages

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

Modifications

- Undo
- Redo

Services

- Calculate

Name:

Comments:

CAPE-OPEN

Calculator

This window helps you to define the context of your thermodynamic calculator

Source type:

Class ID:

Container:

Name:

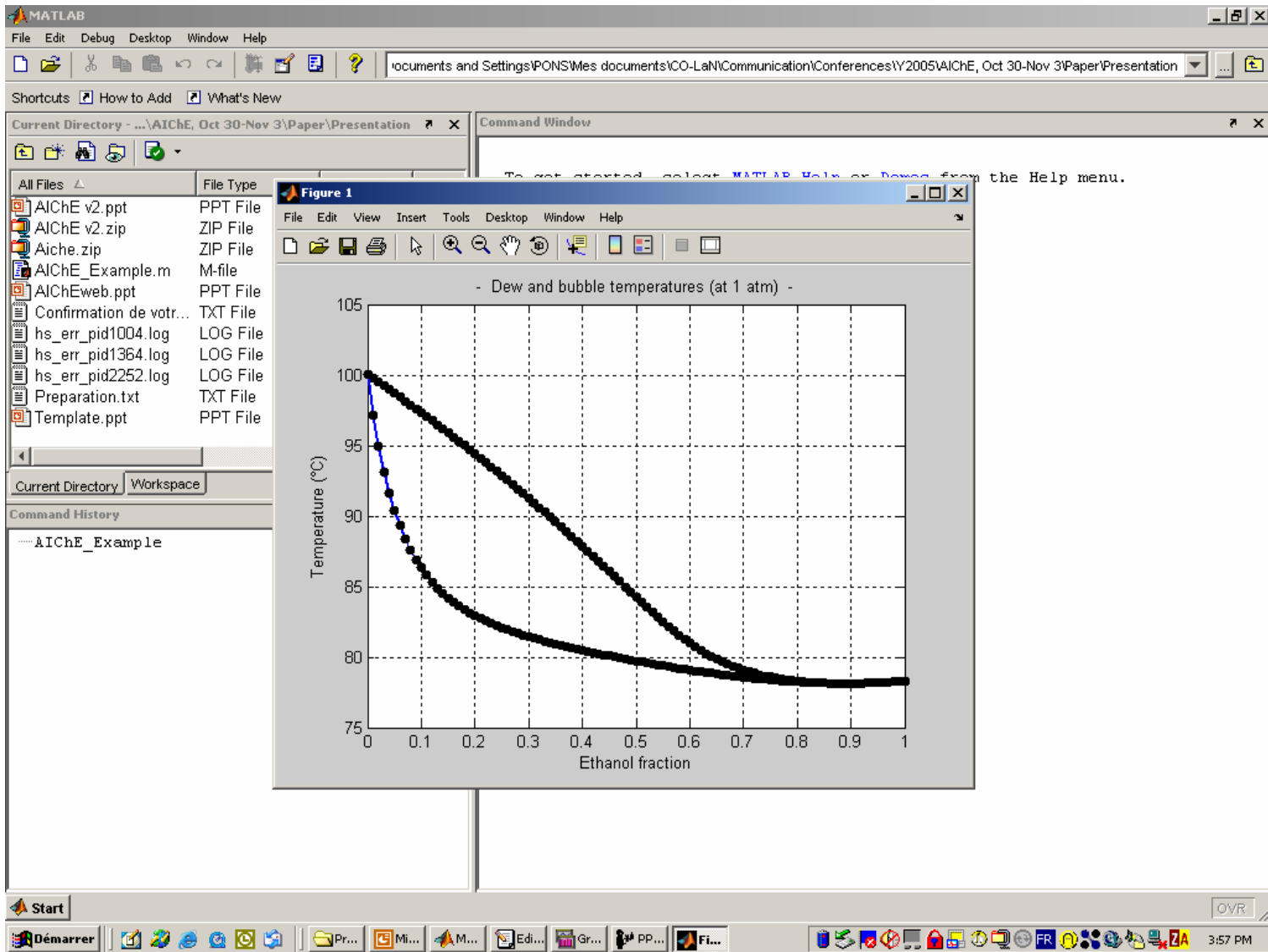
[Details](#)

Ok Cancel

Validate and return to MatLab



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.

