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

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I. Introduction

Throughout their history, process simulation tools had to adapt to the evolutionary nature of hardware and software technologies and to an increasingly demanding market. Usage is again disturbed today by computer networks and co-operative work. In addition to the performance and user-friendliness criteria, the various tools must enable substitution one to another and exchange of services: they must be interoperable and integrable. New technologies based on software components developed with object-oriented languages are available to meet this new market requirement. The CAPE-OPEN standard accompanies that trend by providing a common interface specification for process simulation software.

Considering this situation, ProSim decided to change the architecture of its tools to answer not only its own customers' expectations, but also the whole simulation process software user community. Simulis® project fulfills that goal. Today, three software components are already available. The first one, called Simulis® Conversions, allows to manage quantity and unit conversion in an application. Next, Simulis® Properties, is a pure compound properties server. Properties can be constant or temperature dependent. A pure compound property database, containing more than 1700 compounds, is provided with this software component. The last software component, called Simulis® Thermodynamics, is presented in this paper through its use as a toolbox within MATLAB®. In the future, other components will be developed and will deal with chemical reactions and unit operations.

II. CAPE-OPEN

CAPE-OPEN (CO) is an industry standards on interfaces between pieces of software commonly used in process engineering modeling and simulation activities. CAPE-OPEN standards is supported, enhanced and maintained by the CAPE-OPEN Laboratories Network (CO-LaN), a non-for-profit organization created in 2001. Its missions and organization are described in Belaud et al. (2003). CAPE-OPEN technology widens the application range of any CAPE piece of software and a number of software providers in the CAPE domain have already brought their software to CAPE-OPEN compliance.

CAPE-OPEN standards v1.0 was published at the end of the Global CAPE-PEN project (March 2002). Details of this release are provided by Belaud et al. (2002). These interface specifications were subsequently polished by the CO-LaN in 2003.

CAPE-OPEN facilitates plug and play in CAPE tools, meaning that the same software component (unit operation module, thermodynamic property package, numerical solver) can be used in a number of process modeling environments without having to change any single line of code. Development costs for specialized CAPE tools are consequently reduced while the market for each software component is immediately expanded. There is no need anymore to develop specific interfaces with each other CAPE tool. This facility motivates software developers to migrate their product to CAPE-OPEN compliance in order to retain and achieve market competitiveness.

On the usage side, CAPE-OPEN compliant software tools are providing end-users with an increased capability to choose and use the best tools available for the process engineering objective they have to meet. Including third party software tools in current process modeling environments is made possible, bringing an added flexibility, a larger choice, consequently an improved work process and better results while even reducing cost of process simulation work. Consequently CAPE-OPEN is a technology to widen the application range of any CAPE piece of software. The market leaders in CAPE, a number of niche software providers, as listed by Pons (2003), have adopted CAPE-OPEN, ensuring a widespread usage of the technology.

III. Simulis® Thermodynamics

Simulis® Thermodynamics is a thermodynamic properties and phase equilibrium calculation server for pure compounds and mixtures (containing up to 200 simultaneous compounds). It is based on the well-known ProSim thermodynamic calculation library which has been validated through many years of intensive industrial use. Simulis® Thermodynamics is able to calculate the following properties and their derivatives (with respect to temperature, pressure, number of moles):

- Transport properties (C_p, μ, λ,…).
- Thermodynamic properties (H, S, U,…).
- Compressibility properties (Z, C_p/C_v, …).
- Non-ideal properties (γ, ϕ)
- Pseudo critical properties (T_c, P_c, V_c, Z_c).

And to perform the following phase equilibrium calculations:

- Liquid - Vapor (TP, HP, SP, ωT, ωP, UV, …).
- Liquid - Vapor phase envelope.
- Liquid - Liquid (TP).
- Liquid-Liquid-Vapor (TP, HP, ωP).

Simulis® Thermodynamics model library contains the most used and relevant models as shown in the following non exhaustive list:

- Soave-Redlich-Kwong (SRK),
- Peng-Robinson (PR),
- Lee-Kesler-Plöcker (LKP),

- Benedict-Webb-Rubin modified Starling (BWRS),
- Ideal,
- Wilson,
- NRTL,
- Margules,
- UNIQUAC,
- UNIFAC original,
- UNIFAC modified (Dortmund),
- UNIFAC modified (Larsen),
- PSRK,
- UNIFAC Liquid-Liquid,
- Engels,
- Chao-Seader,
- Sour water,
- Amines and acid gases,
- MHV2,
- ULPDHS,…

IV. Simulis® Thermodynamics and CAPE-OPEN

Even if the Simulis® Thermodynamics architecture is not based, in native, on CAPE-OPEN standard (mainly in order to keep existing codes), Simulis® Thermodynamics proposes a complete interoperability with other software implementing the CAPE-OPEN standard.

On the one hand, throughout its “socket” facility (Fig. 1), Simulis® Thermodynamics allows a client application to calculate properties and phase equilibrium using an external CAPE-OPEN thermodynamic property package coming, for example, from Aspen Properties (AspenTech), PPDS (TUV-NEL), Multiflash (Infochem), ...

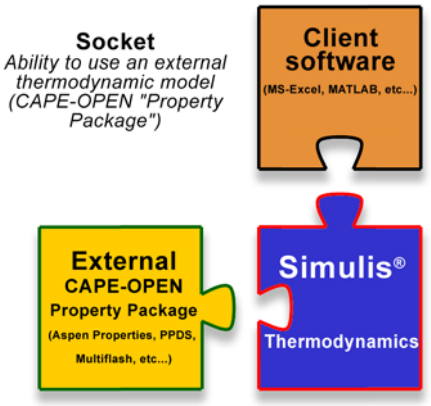

Fig. 1: CAPE-OPEN Thermodynamic "socket" facility

On the other hand, with Simulis® Thermodynamics, an end-user is able to create a CAPE-OPEN thermodynamic Property Package which can be used inside software of other

providers: this is the CAPE-OPEN thermodynamic “plug” facility (Fig. 2). With the help of existing Simulis® Thermodynamics features, a thermodynamic expert can easily build, record and deploy a Property Package to his colleagues. Then, the Property Package can be used in all simulation tools of a company. This functionality has been successfully tested in Aspen Plus® 2004 and v12.1 (AspenTech), Aspen Hysys® 2004 and v3.2 (AspenTech), PRO/II v7.1 (SimSci-Esscor), gPROMS® (PSE) and Xchanger Suite 4.0 (HTRI). Additional testing in VALI (Belsim) and INDISS (RSI) is underway.

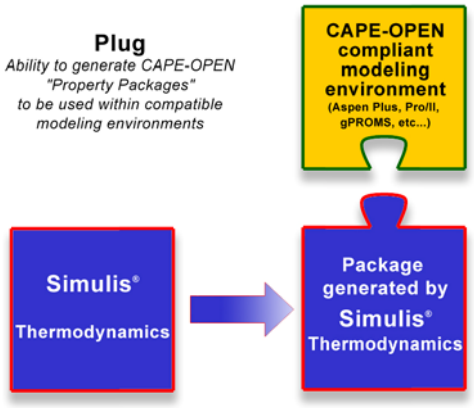

Fig. 2: CAPE-OPEN Thermodynamic "plug" facility

Any application integrating Simulis® Thermodynamics automatically inherits this CAPE-OPEN thermodynamic compliance, both as a plug and a socket.

Finally, as shown on Fig. 3, Simulis® Thermodynamics is always where the end-user needs it and guarantees a true thermodynamic data consistency throughout the different applications the end-user may use.

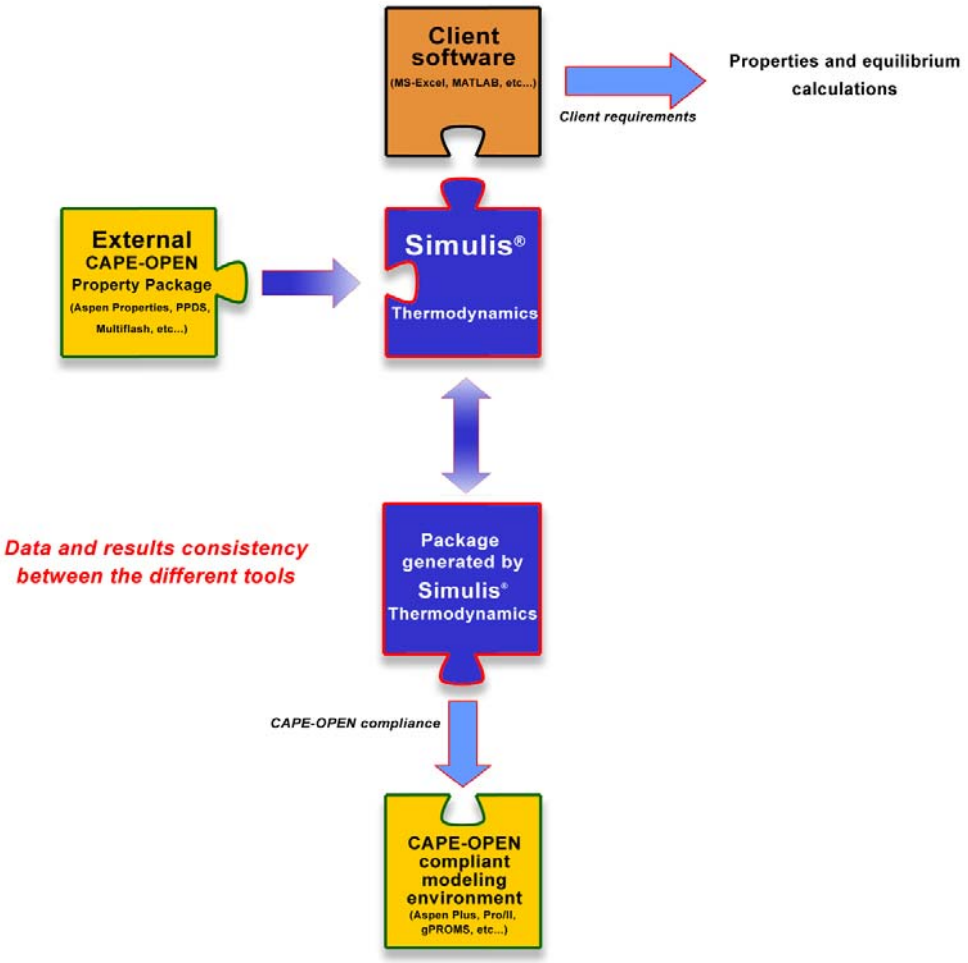

Fig. 3: Simulis® Thermodynamics framework

V. "Integrability" capability of Simulis® Thermodynamics – example within MATLAB®

Now, we are focusing on an important capability of Simulis® Thermodynamics which we call "integrability". One benefit of an architecture based on a component approach is that any application supporting the COM/DCOM technology (and others) can be linked and can interoperate with Simulis® Thermodynamics. The standard commercial packaging of Simulis® Thermodynamics contains a Microsoft® Excel add-in and a MATLAB® toolbox and allows to use it in these environments. A complete API can also be provided and can be programmed easily by using languages such as Visual Basic, C++, Delphi, FORTRAN,…

To illustrate this "integrability" capability, we have chosen an example using the MATLAB® toolbox of Simulis® Thermodynamics (Fig. 4) where a CAPE-OPEN property package is retained to perform vapor heat capacity calculations.

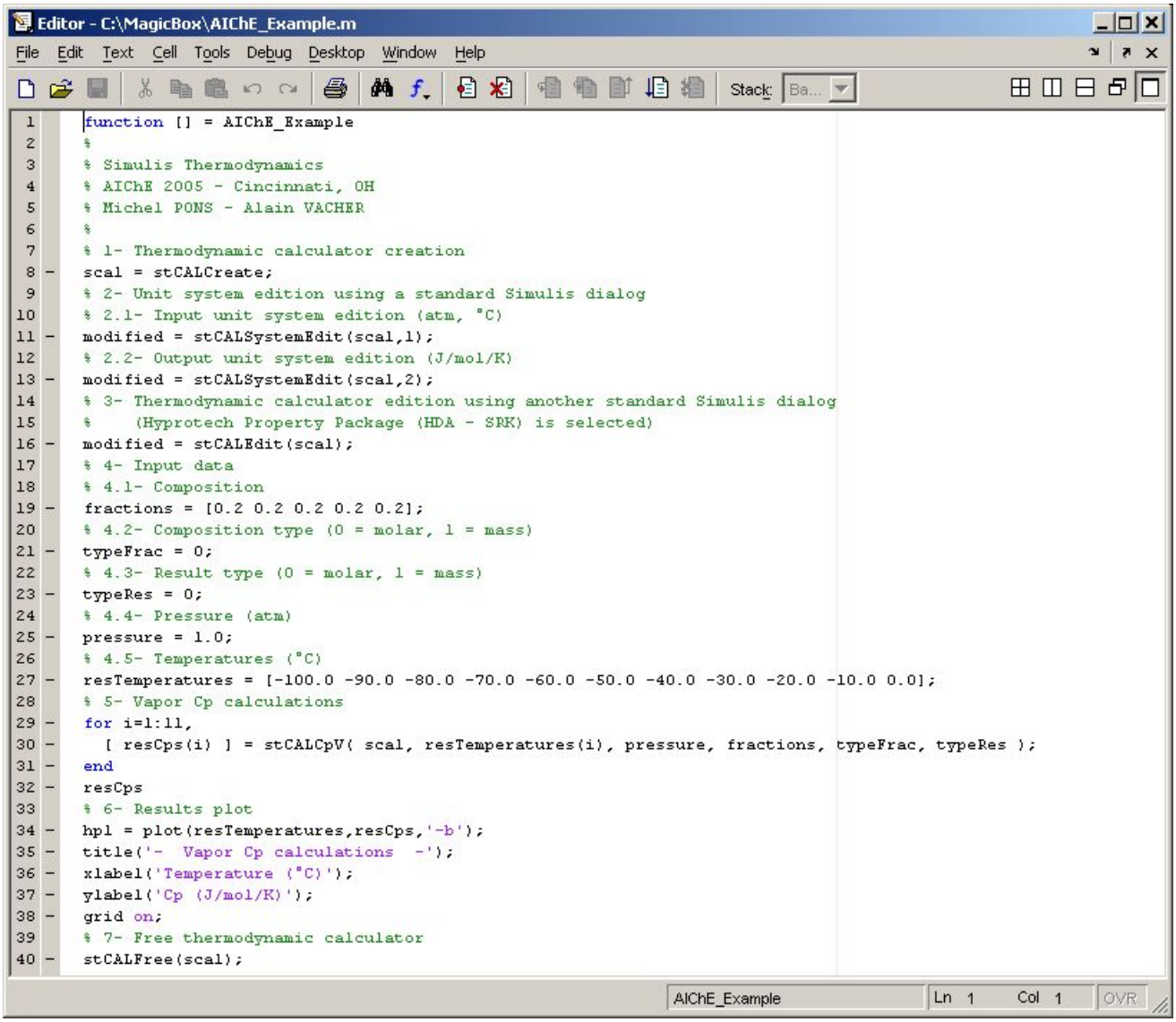

Fig. 4: example of MATLAB® code

The successive steps we can find in this example are the following:

1. Creation of a thermodynamic calculator object used to perform calculations.
2. Edition of its different unit systems (input and output) with a standard dialog (Fig. 5) supplied by the Simulis® framework. In fact, all features of Simulis® Conversions are included in Simulis® Thermodynamics.

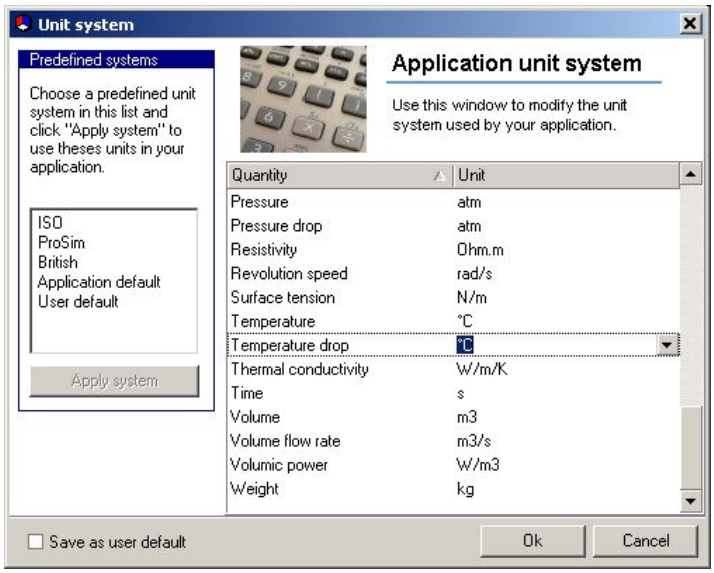

Fig. 5: Unit system edition dialog

3. Edition of the thermodynamic calculator and selection of the CAPE-OPEN Property Package (Fig. 6 to Fig. 8). A thermodynamic calculator in Simulis® Thermodynamics can be described either by selecting a CAPE-OPEN property package or, in native, by importing compounds from different data sources and choosing a thermodynamic model and its related binaries.

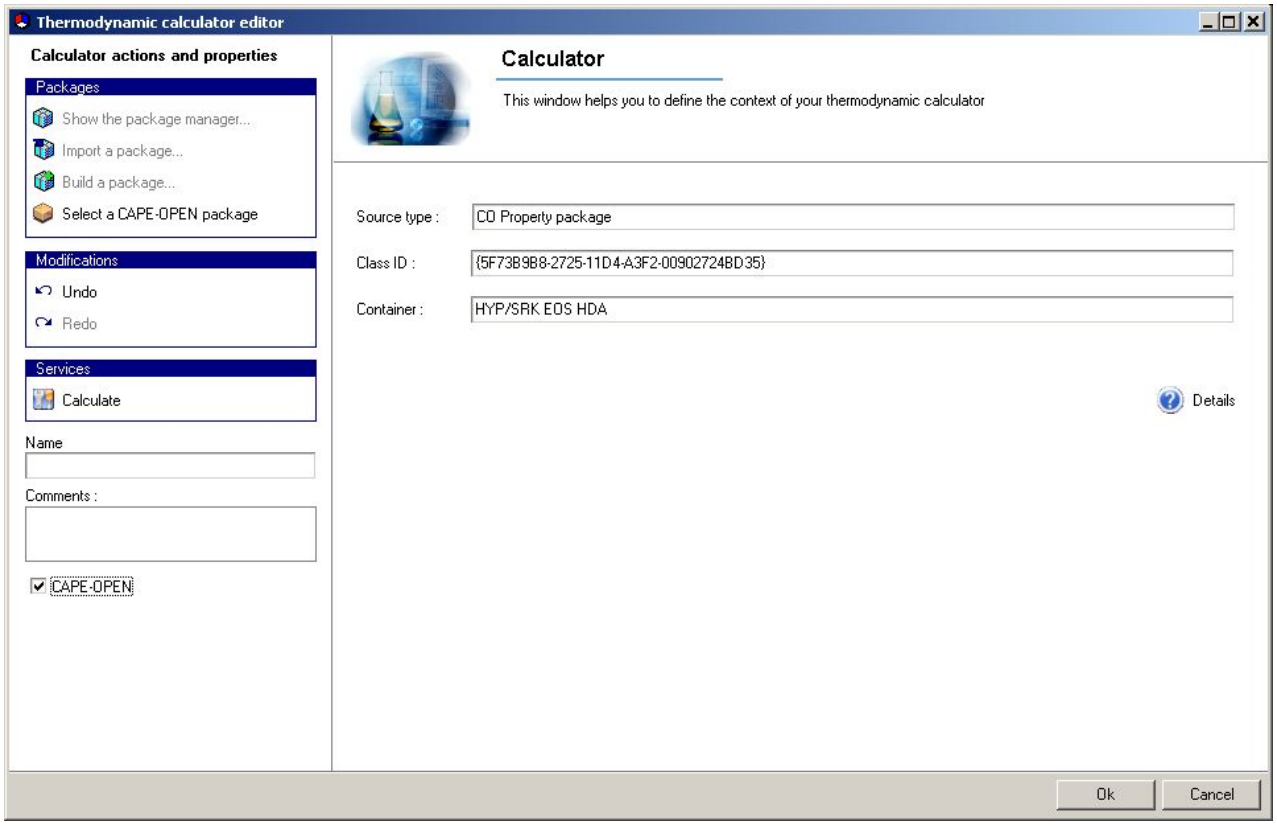

Fig. 6: Thermodynamic calculator edition

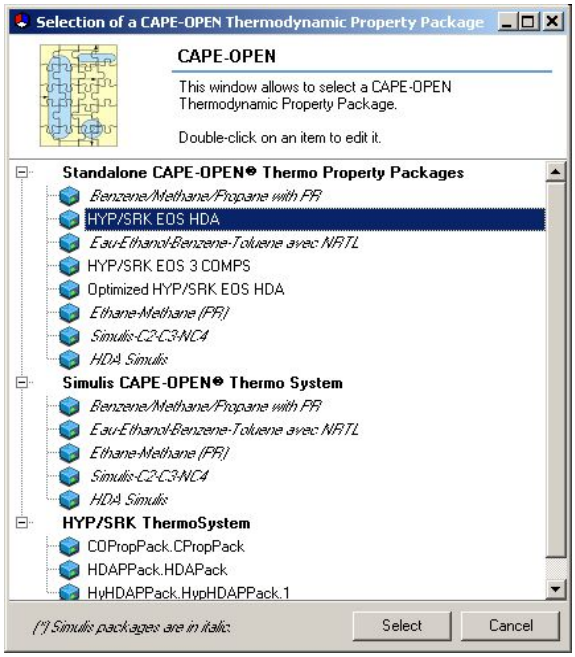

Fig. 7: Property Package selection

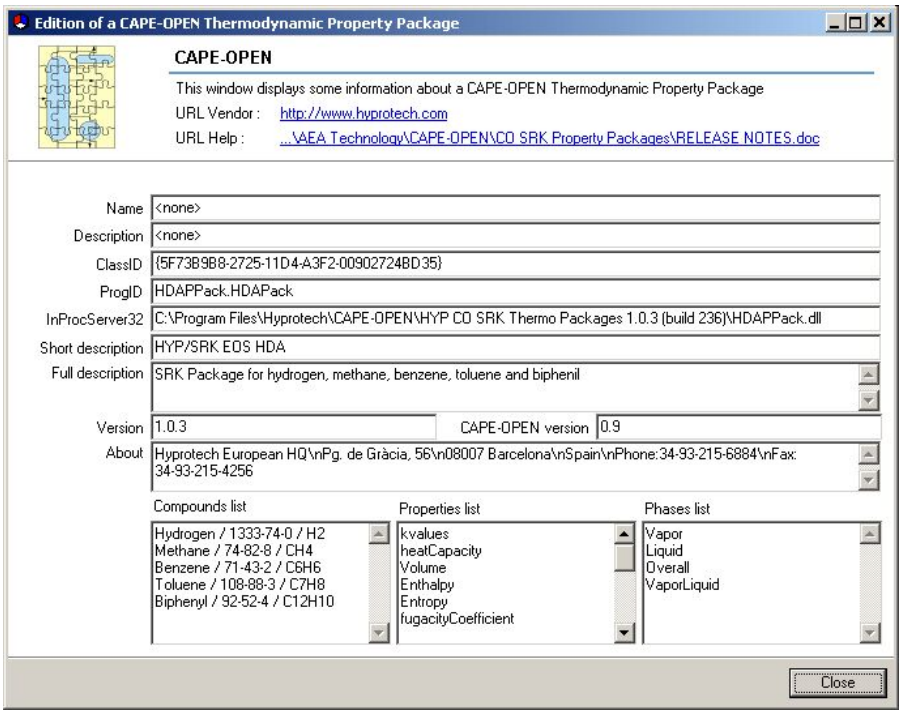

Fig. 8: Property Package edition

4. Input data affectation: range of temperatures, pressure, composition, …
5. Vapor heat capacity calculations.
6. Results plotting (Fig. 9).

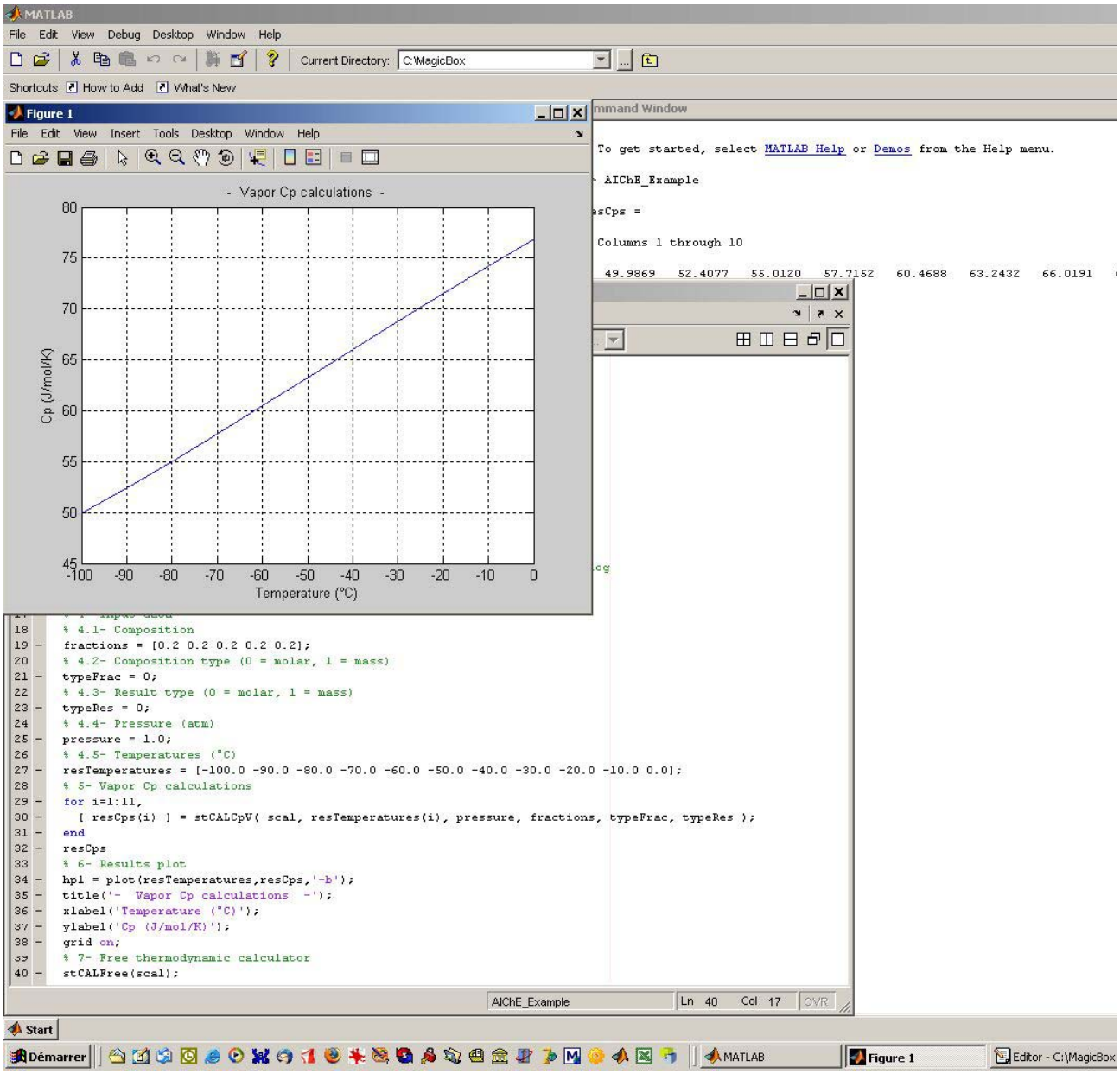

Fig. 9: Plot of the results

7. Release of the thermodynamic calculator.

Over 400 functions of the Simulis® Thermodynamics toolbox allow the programmer to access pure compound properties, thermodynamic models, binaries, CAPE-OPEN property packages and to calculate all available properties and phase equilibrium.

VI. Conclusion

Component based simulation environments open new horizons to study processes. They allow process engineers, by a judicious assembly of ready to use software components, to improve the quality of their studies while reducing associated development times. Thanks to the CAPE-OPEN standard, components interchangeability becomes possible. This flexibility makes it possible to select the software component considered to be most relevant for a given case. Thus, the component approach incontestably brings gains in productivity to the users as well as to the developers of these systems.

VII. References

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