

DEVELOPMENT OF A CAPE-OPEN 1.0 SOCKET

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Introduction

VALI is an advanced data validation and reconciliation software, used online in industry to improve the accuracy of plant data. It is not a simulation software and although process simulation and advanced data validation and reconciliation are similar on several aspects, they are quite different as well. The main difference being the way plant data are handled. In simulation, plant data are used to tune various parameters of simulation models, giving a better model, while in data validation plant data are used to check and correct measurements, giving better information of the actual state of the plant.

Both process simulation and data validation and reconciliation are based on a mathematical model of a process. These models are built using predefined objects modeling the process units operations and the products that are handled. Some information must be available about the physical properties of the chemical components present in the system like their molecular weight, their density, etc.

On the mathematical side, process simulation has been traditionally developed on a modular sequential approach. Each process unit is represented by a mathematical model that calculates the state of the output streams knowing the state of the input streams and some unit operation specifications. Each unit is modeled after the other. When some streams are recycled, convergence algorithms are to be used.

Using such an approach is not possible for data validation and reconciliation. Instead the program must generate equations that relate inputs and outputs. An optimization algorithm is then used to find the set of values that are as close as possible to the measurements while satisfying the equations.

Learning Phase

As a first step of this work, it was important to have a better understanding of both the CAPE-OPEN standards and the COM technology, before even starting the development work. A training course was followed, given by Prosim that has a long experience in implementations of CAPE-OPEN standards.

Cape-open standards

CAPE-OPEN standards are the uniform standards for interfacing process modeling software components developed specifically for the design and operation of chemical processes. The standard defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate. They are based on universally recognized software technologies as COM and CORBA (the two middlewares supported by CAPE-OPEN). The standards are open, multiplatform and available free of charge. They are described in a formal documentation set.

Several versions of the standards are available today:

- 0.9.3: Released in August 2001, this version is still available to support historical applications. It should not be used for any new applications
- 1.0: Released in April 2002. This is the currently supported version.
- 1.1: The official release was made in October 2006.

More information about CAPE-OPEN standards can be found on the CO-LaN Website (www.colan.org). The CAPE-OPEN Laboratories Network (CO-LaN) is the internationally recognized user-driven organisation for the testing and management of the CAPE-OPEN standard. The organisation maintains the list of CO-compliant Software Components.

The complete documentation set of each version of the standards can be downloaded from the CO-LaN Website in a zipped file.

Here are some examples of tools using CAPE models: Steady-state and dynamic simulation, training simulators, data acquisition and reconciliation, optimization of processes, process design tools...

COM technology

COM (Component Object Model) is an interface standard for software components introduced by Microsoft in 1993. It is used to enable inter process communication and dynamic object creation in any programming language that supports this technology. The term COM is often used in the software development industry as a term that encompasses the OLE, ActiveX, COM+ and DCOM technologies.

The main advantage of COM is that it's a language-neutral way of implementing objects that can be used in environments different from the one they were created in. Although the interface standard has been implemented on several platforms, COM is primarily used in Microsoft Environment.

After discussion, Belsim decided to develop the Material Object in .NET C# 2.0. The Material Object is the central point of the architecture and the link between our software and the CAPE-Open Property Package/Thermo Systems. Based on that, two Belsim software have been adapted to be able to create an instance of the Material Object using COM interfaces:

- **ValiModeller**: Graphical User interface designed to model the process. This interface is developed in C++.
- **ValiEngine**: Calculation Engine developed in FORTRAN.

Several COM interfaces in addition to the one defined for CAPE-OPEN have been developed in the Material Object to ease the communication with the calling application.

First Implementation

A first CAPE-OPEN socket version 0.93 was developed in 2001 but the use of a CO-Thermo Package was very difficult for a non-expert user. The Graphical User Interface (ValiModeller) was not able to deal with a third party thermodynamic model and we had to use a text editor to define a thermo plug. Furthermore, the compliance was not complete because Vali did not use the actual compounds of the CO-Thermo Package for all the calculations. Having had this experience, eased the development work of a CAPE-OPEN 1.0 socket.

Development Phase

The Material Object (MO)

The Material Object is the communication interface between the PME (Process Modeling Environment) and the PMC (Process Modeling Components). In the CAPE-OPEN 1.0 architecture, the Material Object is implemented at the PME level. In the case of our development (Thermo Socket), the Material Object was the central point of the architecture and the link between Belsim Software and Thermo Plugs making crucial this part of the system.

It was decided to develop a proprietary Material Object in C# 2.0 using Visual Studio 2005. According the specifications of CAPE-OPEN 1.0, the Material Object developed by Belsim implements the interface "ICapeThermoMaterialObject". All Methods defined in this interface have been implemented.

Cape-Open thermo plugs viewer

The first graphical tool to be developed was a small tool based on COM technology to allow the user to see what Thermo Systems and Property Packages are available on a given computer. This tool has been developed in C# 2.0 using Visual Studio 2005.

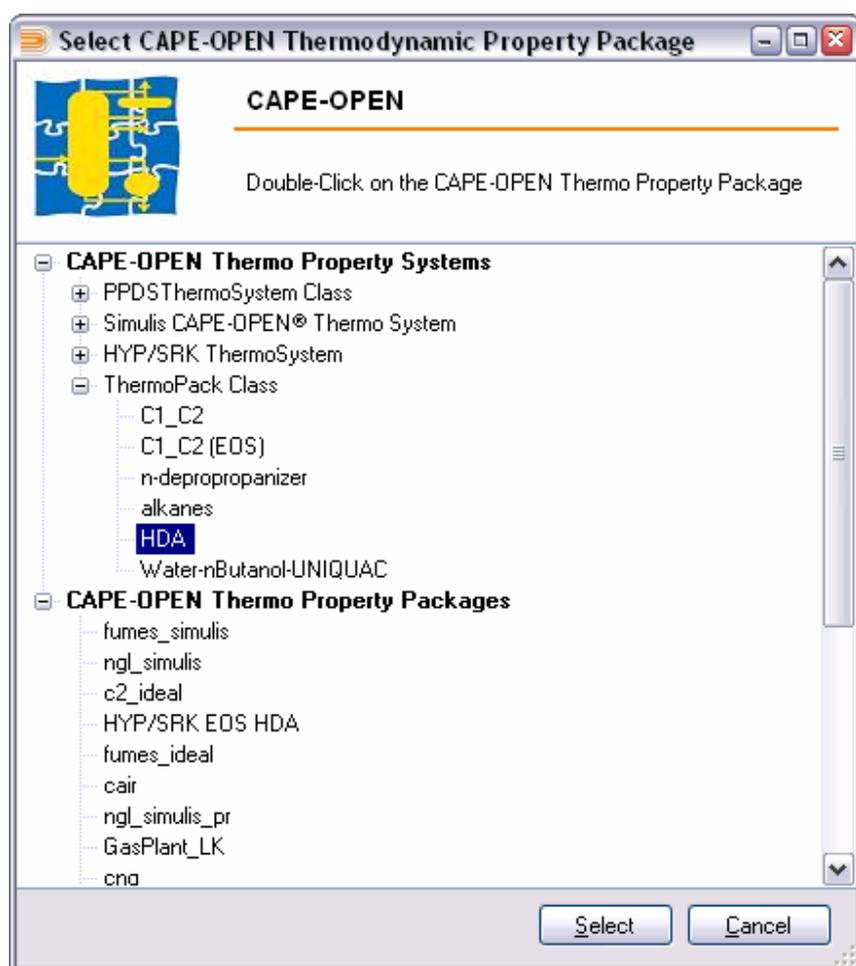


Figure 1: Example of interface listing thermodynamic packages available

Graphical user interface (ValiModeller)

ValiModeller is the Graphical User Interface in the suite of VALI software. It is developed in C++. When defining a validation problem you need to choose a thermodynamic package (list of compounds, list of thermodynamic methods and if you have binary parameters). In ValiModeller the option of choosing between Belsim's own thermodynamic package or a CAPE-OPEN package has been integrated.

The user needs to select between the following options:

- Build a thermodynamic package from existing integrated databases of compounds and Thermodynamic methods (called native thermo and compounds).
- Select a Cape-Open 1.0 Thermo Property Package available on the computer. The selection is made through the viewer shown here above.

ValiModeller is also able to list the compounds and properties available in the CO-Thermo Package.

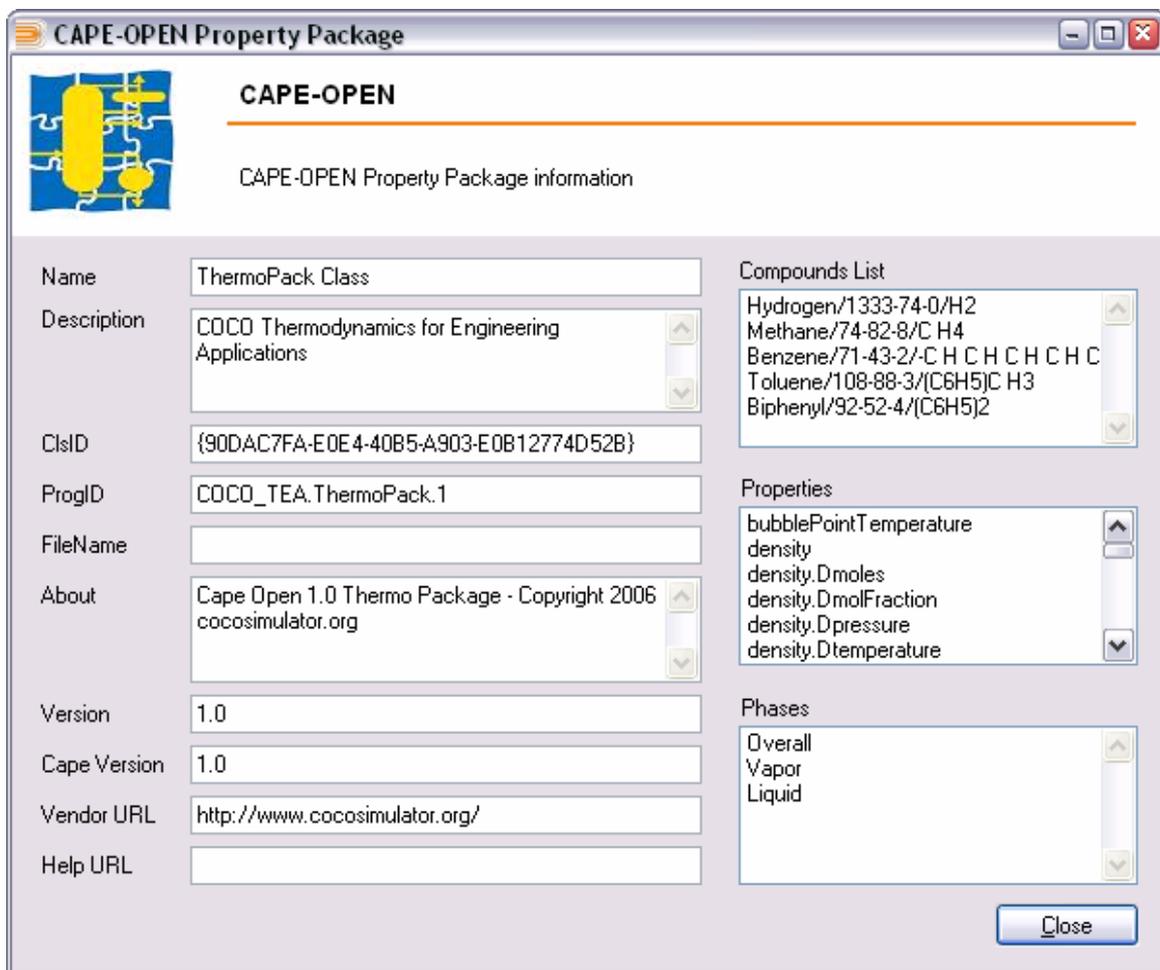


Figure 2: Example of interface listing information of a property package

The information shown in this window is collected from the Property Package through the Material Object (MO).

Vali Engine

In a first step, it was necessary to verify that everywhere in the code when a pure compound property is needed, the property is given by the Thermo Package (through the MO) and not by an internal calculation. These properties are:

Name, Chemical Formula, CAS number, Molecular Weight, Boiling Temperature, Enthalpy of Formation.

After that, the different routines used to calculate a given property of a mixture have been modified to get the result of the calculation from the Thermo Package and not from a Vali internal routine. Here are the following properties: Liquid and Vapor Enthalpy, Volume, Entropy, Gibbs' Free Energy, Viscosity, Conductivity and Fugacities (or Fugacity Coefficients or Activity Coefficients).

The choice to calculate flashes directly from the Thermo Package (optional) or to calculate them using the internal routines with the Properties listed above coming from the Thermo Package is also available.

Testing Phase

Process Description

We have chosen the well known hydrodealkylation (HDA) process to test CAPE-OPEN 1.0 thermo plug. Data come from sample flow sheets available on COCO (cape open to cape open) internet site (http://www.cocosimulator.org/index_sample.html)

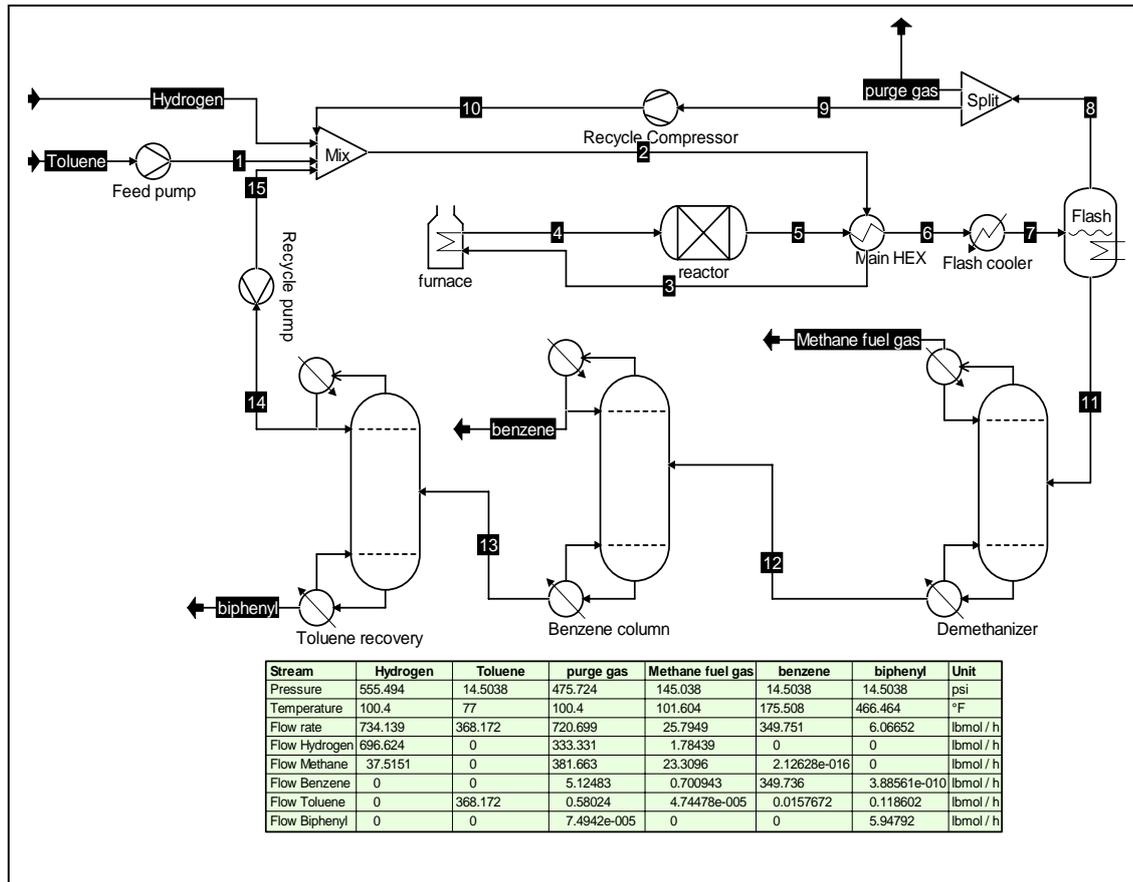
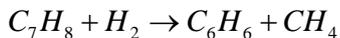
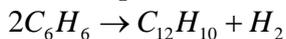


Figure 3 : HDA process (COFE software)

HDA process converts toluene to benzene. The main reaction path is:



Benzene produced is involved in a side reaction:



The reactions proceed irreversibly without a catalyst at temperature in the range of 1200-1270°F with approximately 75% of the toluene gas converted to benzene and 2% of the benzene produced in the HDA reaction converted to biphenyl. The reactions occur in series in single processing unit.

HDA process is presented in figure 3 (The figure is a printed view of the COFE software).

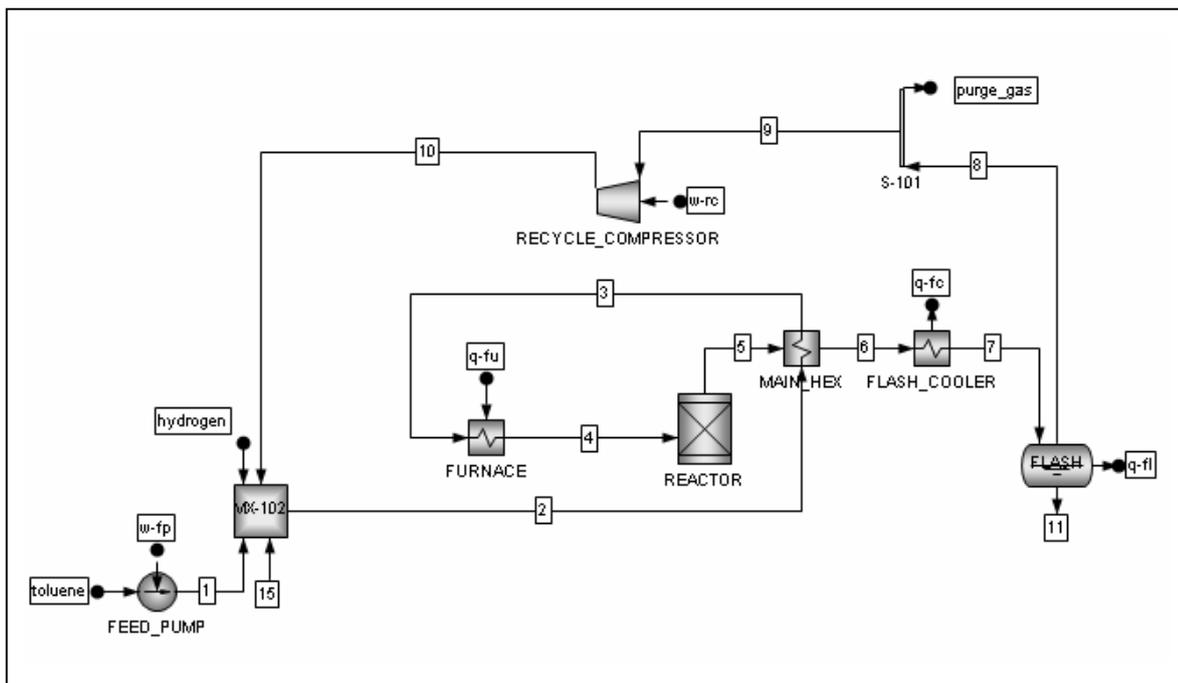


Figure 4 : Reaction section (VALI software)

Process simulation with VALI

The process has been modelled with VALI software using its own (we call it native) thermodynamic database of chemical compounds (to define hydrogen, methane, benzene, toluene and biphenyl) and methods (the classical SOAVE equation was chosen). It has been divided in two main sections: reaction and distillation. The resulting graphical user interface is presented in figures 4 and 5.

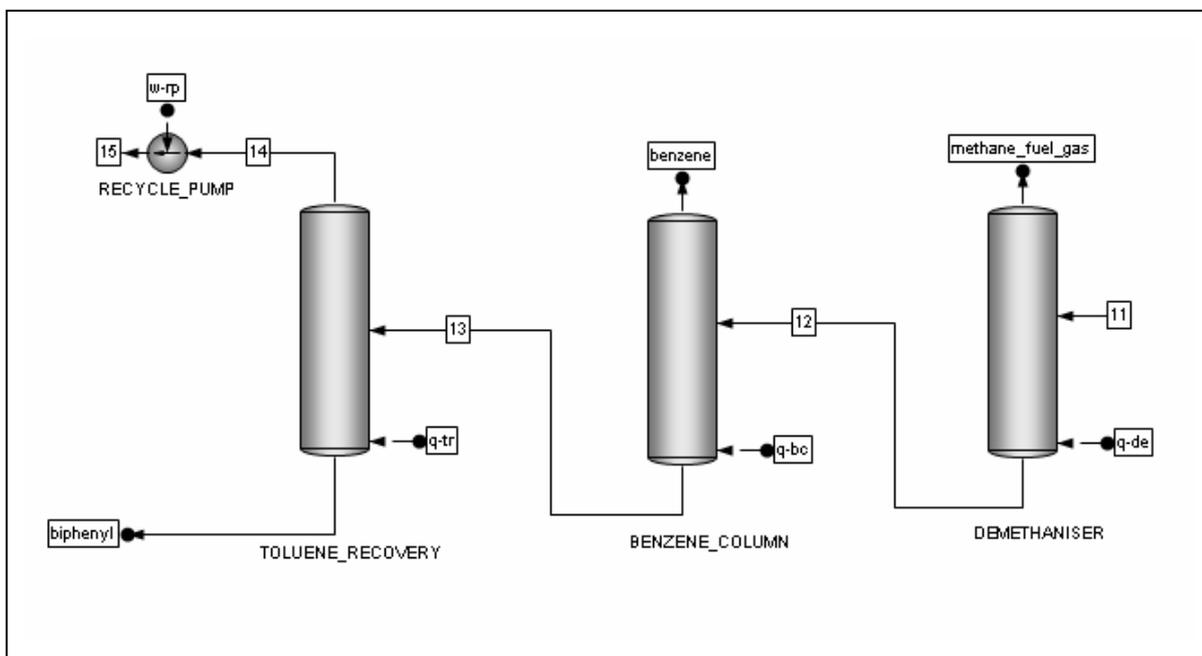


Figure 5 : Distillation section (VALI software)

Process simulation with VALI and CAPE-OPEN thermo plugs

The next step was to substitute the native thermodynamic models with different imported CAPE-OPEN thermo plugs.

The first one was a “COCO Thermodynamics for Engineering Applications” called “COCO_TEA.ThermoPack.1” containing the same compounds and a modified SOAVE-REDLICH-KWONG equation.

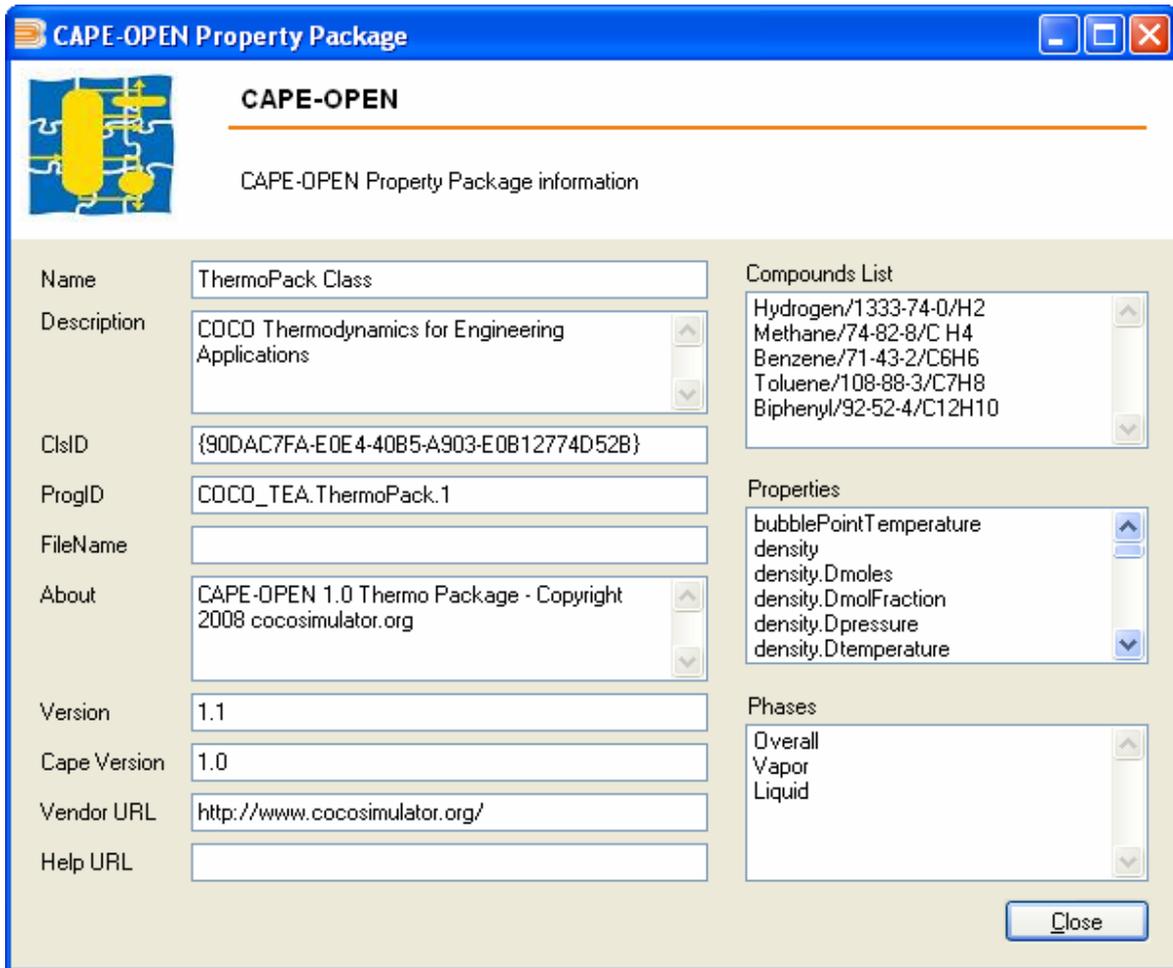


Figure 6 : interface listing information of HDA property package of COCO

The second one was a Simulis package containing the same compounds and a classical SOAVE-REDLICH-KWONG equation.

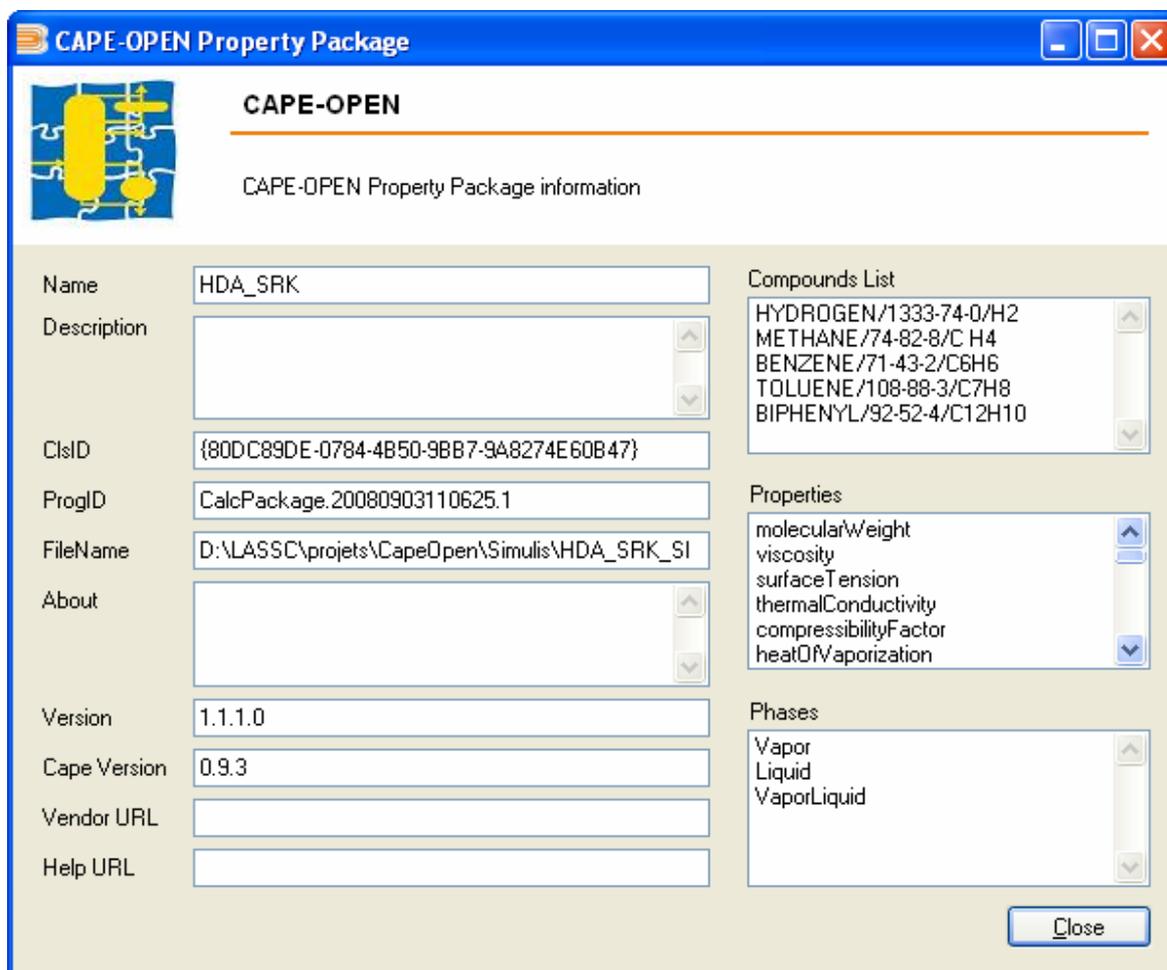


Figure 7 : interface listing information of HDA property package of Simulis

Simulation results with VALI native and CAPE-OPEN thermo plugs

The simulation results were similar with 349.6 klbmol/hr benzene and 5.94 klbmol/hr biphenyl productions from 368 klbmol/hr toluene input. The flash conditions were computed identical at 100 F and 475.5 psia.

The CPU time consumed for the different computations was depending on the thermo plug type. The verification phase was speedier with the native one and much slower with the simulis one. The resolution phases were similar.

Table 1. CPU Time and Number of Iterations Comparison

	Verification	Resolution	Total	Iterations
Native	0.71	3.63	5.69	4
Coco	3.14	3.42	8.38	5
Simulis	5.75	2.66	10.56	3

Verification phase implies loading all the necessary data and physical property model, and checking that all required properties can be calculated.

In the resolution phase, mass and energy balance equations were solved, as well as specifications handled as pseudo measurements.

In this case, the number of specified measurements was such that the problem was just calculable (no redundancy). The number of iteration needed to solve the problem with the prescribed accuracy differs slightly according to the thermo system used, even if the same equation of state was selected in all cases. We expect that the convergence criterion in the solution of the equation of state was not the same in all cases which may have an impact on the speed of convergence in the outer loop.

Conclusion

Using a thermo socket is time consuming during the verification phase certainly to access the corresponding “dll” file. However it seems that the time required to perform one iteration is approximately the same for the native thermo or for the CAPE OPEN plugs.

Similar test has been done with the Cavett’s problem with similar conclusions.

General Conclusion

These developments were time consuming and especially estimating the time needed for the development was difficult. Testing and Debugging were also rather challenging because all the thermo plugs were not available on the same computer as our source codes. To conclude, VALI has today a CAPE-OPEN 1.0 socket that has been successfully tested on several different CAPE-OPEN 1.0 thermo plugs.