Towards the Standardisation of Thermodynamic and Physical Properties Packages

Benqlilou[1] C., S. Bel[1], M. González[1], M. Pons[2], R. Szczepanski[3], A. Espuña[1], and L. Puigjaner[1]

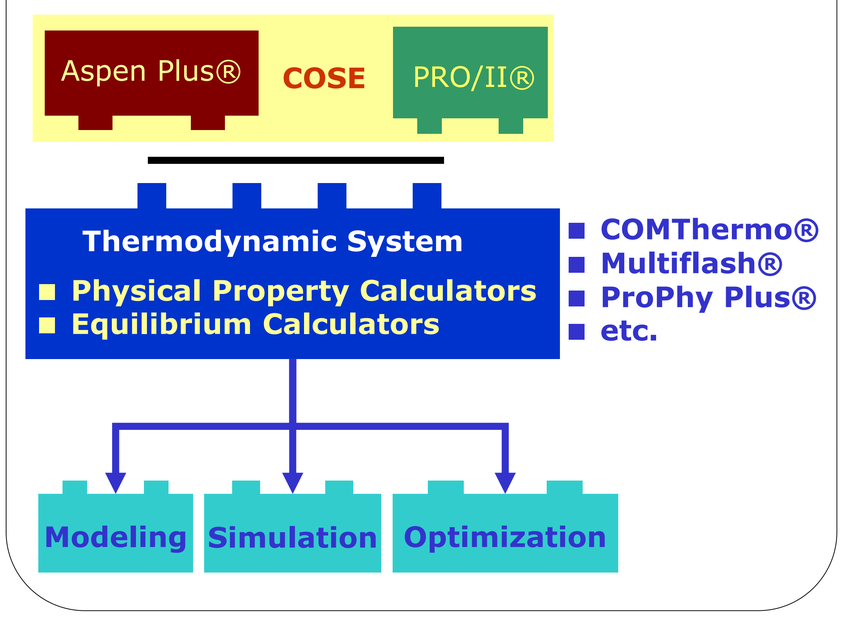
[1]Universitat Politècnica de Catalunya, Chemical Engineering Department,
Av. Diagonal 647, E-08028 – Barcelona (Spain)
[2]ATOFINA Centre Technique de Lyon BP 32 69492 Pierre-Benite Cedex, France
[3]Infochem Computer Services Ltd., 13 Swan Court, 9 Tanner Street, London, SE1 3LE, U.K.

14th ESCAPE, Lisbon 2004

Adapting of a Thermodynamic and Physical Properties (Thermo) Package to the increasing improvements of computer performance and the development of new, efficient, and robust thermodynamic methods, remains expensive in time, cost and implementation effort. An efficient solution to overcome these drawbacks is to standardise Thermo communications with client applications in a consistent, efficient and secure way by designing a well-defined interface that ensures interoperability and transparency. The CAPE-OPEN (CO) standard provides such a facility. To enhance the existing standard, a revision of the CAPE-OPEN Thermo interface specification (version 1.1) has been proposed. A thermodynamic package has been wrapped to comply with this interface specification using COM technology.

Considered as a help to developers, a Tester to verify compliance with the standard has been specified and developed. This Tester, a part of the CO-Tester suite, will be freely distributed and used to validate the consistency and compliance of the pieces of software implementing the new version of the CO Thermo interface specification.

Thermodynamic Systems



Plug & Play problems

- **Cost**
- **Implementation effort.**
- **Diversity of functionalities and interfaces of each tool**
  - **data conversion**
  - **interfaces mapping**
  - **unsafe information transfer**

Cape-OPEN provides an open and flexible Thermo standard interface that overcomes these issues

This standard facilitates plug and play capabilities, which in turn motivates the software developers to wrap their product in order to increase their market share (e.g. HYSYS®). CAPE-OPEN is an enabling technology for including third party tools in other applications.

Motivation for version 1.1

Experience with integrating Thermo 1.0 in Integrated environments

- **Extension** (Multi-phase calculations, accommodate specialist equilibrium calculation tools, whose capabilities go beyond those of typical commercial simulators.)
- **Simplification** (less methods which are logically grouped in interfaces to remove duplication leading to cleaner and more abstract design)

Increased flexibility
Improved efficiency
Removal of ambiguities

Overall Design

The Thermo interface specification highlights four main areas of services

Physical Property Calculator (PPC) — determines value of a set of non-constant physical properties of some material at a given T, P, C and within a given phase.

Equilibrium Calculator (EC) — the composition and amounts of each phase of a material subject to specified constraints such as a PT flash.

Property Package (PP) — is a software component that combines the functions of a PPC and an EC for a fixed set of compounds and phases.

Property Package Manager (PPM) — a software component that manages a set of PPs. It is responsible for instantiating PPs on request and may allow PPs to be edited and/or created.

Material Object (MO) — exposes all the Thermo interfaces and it is responsible for holding the data and providing access to the value of the properties that describe the state of the material. Thus, MO is the central component of the Thermo system architecture

The client could be any application (e.g. PME CO-Tester)

Prototyping Thermo 1.1

In order to validate the adequacy and operability of the interface specification, a prototype is developed to act as a feedback for clarifying and improving the specification.

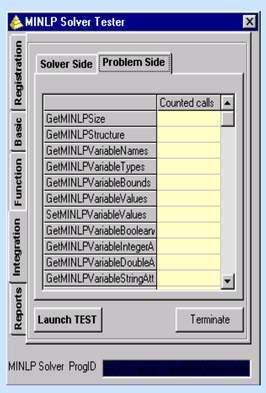
The Property Package provides a thermodynamic model, a cubic equation of state (RKS), which calculates volumetric properties, thermal properties and fugacity coefficients.

Additional models for gas and liquid viscosity are also provided within the package. To test the multiphase features of the interface, three phases are supported (vapour, liquid and aqueous liquid).

The Thermo interfaces and methods are developed in Visual Basic 6.0 to facilitate rapid prototyping and wide usability.It is worth mentioning that the calculation engines are implemented as independent Windows DLLs.

In order to check if the Thermo 1.1 prototypes comply with Thermo 1.1 interface specification, a Tester is required. This Tester aims to help software providers to develop components that are CO-compliant.

CO Tester



The CO Tester acts as a basic simulation environment where software components can be plugged in. It has been designed to automatically carry out a number of scenarios. First, the CO Tester checks for the existence of the required CO interfaces within the tested software. This constitutes the Basic test. Then each method of each interface is tested on its arguments (existence and type), and on its functionality. This constitutes the Function test. Any developer is also able to run self-designed tests through the Integration test part, where the developer defines the test scenarios.

The CO Tester prepares a report which enables any developer to assess the compliance of a piece of software with the CO interface specifications.

Conclusions

Benefits for suppliers
- Reduced development costs
- Increased usage of CAPE tools

Benefits for users
- Develop once, run everywhere
- Access to best-in-class solutions

Benefits for academics
- Improved dissemination of research results
- Better adaptation to industrial needs