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Next Generation Computer-Aided Process Engineering
Open Simulation Environment

Project Coordinator: IFP - Institut Français du Pétrole
Partners:
BASF, BAYER, BP, DUPONT, ELF, ICI
RWTH.LPT, RWTH.IS, ICSTM, INPT
ASPENTECH, HYPROTECH, SIMSCI, QUANTISCI

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CAPE-OPEN
Next Generation Computer Aided Process Engineering Open Simulation Environment

Synthesis Report

The CAPE-OPEN Consortium

CO-MGT-IP-24 Version 3

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2. Summary

2.1 Keywords :

Process Simulation, Computer-Aided Process Engineering, Standard Interfaces, Thermodynamics and Physical Properties, Unit Operations, Numerical Solvers

2.2 Abstract of the results and benefits of the project

Fast, accurate, and effective process modelling is increasingly vital for the synthesis, design, monitoring and optimisation of chemical and related processes. Different simulators have different strengths, so that to obtain the best results for a particular problem, access to more than one vendor simulator and to in-house software containing company specific methods or data is usually required. For this reason, the EC sponsored the CAPE-OPEN project, which aimed to develop, test, describe and publish agreed standards for interfaces of software components of a process simulator. The main objective was to enable native components of a simulator to be replaced by those from another independent source, or that are part of another simulator, with minimal effort in as seamless a manner as possible.

On completion of the project, prototypes of CAPE-OPEN compliant software components have been developed, tested and demonstrated. They prove that it will be possible to assemble a process model from a set of software components encapsulating physical property methods, unit operation models and numerical algorithms. It is possible for these components to be newly developed software or wrapped legacy code that are communicating through the open standard interfaces.

CAPE-OPEN delivered interface standard specifications for the main components of a process simulation, as described above. These will be further developed and expanded through the forthcoming Global CAPE-OPEN project.

The major deliverable of CAPE-OPEN is the set of interface specifications documents together with their accompanying explanations. These are made available as HTML and pdf files on the CAPE-OPEN web site. They are:

- CAPE-OPEN Roadmap
- CAPE-OPEN Concepts
- Thermodynamic and Physical Properties Open Interface Specifications
- Unit Operations Open Interface Specifications
- Numerical Solvers Open Interface Specifications
- Sequential Modular Specific Tools Open Interface Specifications
- Simulator Executive Specifications
- Report on Validation
- Report on PATH Research

The set of documents delivered by CAPE-OPEN shows how CAPE-OPEN will fundamentally impact the future of process simulation in the next decade. The fact that these documents were produced by a consortium gathering highly competitive software suppliers, some of their major customers, and a group of world-famous research laboratories, is in itself a significant result and a proof that standardisation of software components interfaces for process simulators is achievable and should be continued.

3. The Consortium

3.1 Partner organisations

AspenTech UK Ltd
Dr Rob Noble
Sheraton House
Castle Park
Cambridge CB3 0AX
441223312220
441223366980
UK
noble@atuk.aspentec.com

BASF Aktiengesellschaft
Mr Hans-Horst Mayer
ZIC/I
L511
D-67067 Ludwigshafen
49 621 60 56097
49 621 60 56030
Germany
hans-horst.mayer@basf-ag.de

Bayer AG
Dr Stefan Artlich
Process Technology/Applied Mathematics
ZT-TE 2, Bld K9
D-51368 Leverkusen
49 214 3062291
49 214 3064801
Germany
stefan.artlich.sa@bayer-ag.de

BP International Limited
Mr Peter Banks
Process Simulation
Research and Engineering Centre
Chertsey Road, Sunbury on Thames
Middlesex TW16 7LN
44 193 2764458
44 1932763952
UK
peter.banks@which.net

DuPont Iberica
Dr Juan Carlos Rodriguez
JuanCR@hyprotech.com

Elf Atochem
Dr Michel Pons
CRDE
BP6 1005
57501 St Avold Cedex
33 87 91 78 57
33 87 91 78 47
France
michel.pons@crde.elf-atochem.fr

Hyprotech
Mr Salvador Clavé
Pg de Graci, 56
08007 Barcelona
34 93 215 6884
34 93 215 4526
Spain
SalvaC@hyprotech.com

ICI
Dr Tom Malik
Technology Manager -Process Modelling
PO Box 8
The Heath
Runcorn WA7 4QD
44 1928515603
44 1928515660
UK
Tom_Malik@ici.com

Imperial College
Pr. Costas Pantelides
Centre for Process Systems Engineering
LONDON
SW7 2BY
LONDON
44 1715946622
44 171 5946606
UK
c.pantelides@ic.ac.uk

INPT-ENSIGC
Pr. Xavier Joulia
Laboratoire de Génie Chimique
18, Chemin de la Loge
F-31078 Toulouse Cedex 4
33 5 62 25 23 55
33 5 62 25 23 18
France
Xavier.Joulia@ensigct.fr

Institut Français du Pétrole
Dr Bertrand Braunschweig
Computer Science and Applied Mathematics
1 & 4 avenue de Bois Préau
92500 Rueil Malmaison
33 1 47 52 66 48
33 1 47 52 70 22
France
Bertrand.Braunschweig@ifp.fr

Enviros QuantiSci
Dr Michael Williams
Chiltern House
45 Station Road
Henley-on-Thames, Oxfordshire RG9 1AT
44 149 1410474
44 149 1576916
UK
michael.williams@enviros.com

RWTH Aachen. I5
Pr. Matthias Jarke
Lehrstuhl Informatik V
Ahornstrasse 55
D-52056 Aachen
49 241 80 21500
49 241 88 88 321
Germany
jarke@informatik.rwth-aachen.de

RWTH Aachen. LPT
Pr. Wolfgang Marquardt
Lehrstuhl für Prozesstechnik
Turmstrasse 46
D-52056 Aachen
49 241 80 67 12
49 241 88 88 326
Germany
maq@lfpt.rwth-aachen.de

Simulation Sciences
Mr Heeren Pathak
SIMSCI Ltd.
Highbank House
Exchange Street
Stockport, Cheshire SK3 0ET
United Kingdom
Telephone: +44 161 429 6744
Facsimile: +44 161 480 9063
Hpathak@simsci.com

3.2 Consortium Description

IFP

IFP pursues a wide range of research and development, training, information activities, and industrial development, servicing the complete chain of petroleum operations, ranging from exploration to the many uses of petroleum products, and including environmental problems. IFP is a major process licensor with over one thousand licensed issued, with leading positions in the refining and olefins business.

IFP was the project co-ordinator, chair of the Steering Committee, of the Methods and Tools group, and contributed to all tasks including development of software test harnesses and prototypes. It was represented in the project by senior researchers from the Computer Science and Applied Mathematics Department, from the Process Engineering Department, and from the Applied Physicochemistry and Analysis Departments.

BASF Aktiengesellschaft

BASF AG is a chemical company operating world-wide and ranks among Europe's top chemical companies. Most of the plants for these products are and will continue to be developed and optimised by the Engineering and the Research Departments at Ludwigshafen. A core tool for this task is flowsheet simulation, and flexible in-house process simulation software has been used extensively.

BASF was a member of the Steering Committee, the leader of the Thermodynamics and Physical Properties work package and contributed to interface specifications.

BAYER

Bayer is an international, broadly diversified chemicals and health care company with operations in some 150 countries. Product areas are pharmaceuticals and health care products, polymers, organic products, industrial products and agrochemicals.

BAYER was a member of the Steering Committee, the leader of the Validation work package, and contributed to several interface developments mainly in Thermodynamics and Numerics.

DUPONT

Dupont is a broad based manufacturer and supplier of chemicals and related materials. The product areas include chemicals, polymers, agrochemicals, imaging systems and medical products. Process simulation is vital to achieving DuPont's environmental reduction programmes and enhancing the capabilities of their operations throughout Europe.

DUPONT was a member of the Steering Committee, chair of the Exploitation Committee, the leader of the PATH workpackage, and an active member in several technical activities, including Unit Operations, Methods and Tools, Documentation. DuPont produced the first component-based testbed environment for process simulation in the PATH work package.

ELF AQUITAINE

Elf Aquitaine is one of the French leading industrial groups in terms of sales, income, and international scope and operations. One of the ten largest oil and gas and chemical companies world-wide, Elf controls some 750 companies in over a hundred countries. Elf's activities continue to develop around its three major divisions: Oil & Gas, Chemicals and Healthcare.

Elf was a member of the Steering Committee, the leader of the Numerical work package, and an active member in several technical areas, including Numerics, Methods and Tools, Documentation, and the setting up of the CORBA software demonstration.

ICI

ICI is one of UK's leading technologically based industrial companies and one of the world's foremost chemical companies. The company has a long history of innovation both in process technology and supporting engineering technology.

ICI was a member of the Steering Committee, chair of the Scientific and Technical Committee, and the leader of the Conceptual workpackage, and a reviewer for all technical activities. ICI also co-ordinated the Documentation effort.

BP INTERNATIONAL

BP is a major multinational oil and petrochemical group that has been actively involved with process simulation since the early 1960's and is now a significant user in all the main areas of its business.

BP's contribution to the project was being co-ordinated from the Group Research and Engineering Centre, which is where the in-house simulator is supported.

BP was a member of the Steering Committee, the leader of the Unit Operations workpackage, and an active member in several technical areas, including Unit Operations, Documentation, and the setting up of the COM software demonstration

RWTH AACHEN.LPT

The Lehrstuhl für Prozeßtechnik has been founded by a joint initiative of Bayer AG and RWTH Aachen on November 1, 1992 as part of the Department of Mechanical Engineering. The research program of the Lehrstuhl für Prozeßtechnik aims at covering different issues in process systems engineering. The focus is on fundamentals of as well as software tools for a model-based design of chemical processes and their application to relevant industrial sample problems.

RWTH.LPT was a member of the Scientific and Technical Committee, an important technical contributor to all work packages with a special emphasis on PATH, Validation and Conceptual activities. RWTH developed the CHEOPS CORBA-based workbench which was the integration platform for the CORBA demonstrator.

RWTH AACHEN.I5

The Information Systems research group focuses on theoretical analysis, prototype development, and practical evaluation of meta information systems. It has experience with various approaches to system interoperability and re-engineering. It also has long-term experience of prototype systems for supporting the process of model generation and evolution and experience of running an Internet based information server for various projects and groups.

RWTH.I5 was a member of the Scientific and Technical Committee, contributed to the project in component based application building techniques, especially enriching and selection of comports, platform inter-working, code migration, and in establishing the project specific software process along with training the project partners.

IMPERIAL COLLEGE

IMPERIAL COLLEGE researches all aspects of process design, operation, control and modelling. It currently employs more than 100 researchers and has substantial expertise in the design and implementation of process modelling tools, making it a valuable partner for the development of an open simulation environment.

IMPERIAL COLLEGE was a member of the Scientific and Technical Committee, a major technical contributor in the Conceptual and Numerical work packages (principal author of the Solvers interface), and a reviewer in other activities. Imperial also contributed a component for the CORBA demonstrator in addition to the software prototypes for the Numerical Workpackage.

INP TOULOUSE-ENSIGC

The INPT/ENSIGC research activities are carried out by 16 teams grouped in the “Institute de Génie des Procédés”. Some teams are associated with the CNRS (National Science Research Centre). ENSIGC currently has 120 doctoral students supervised by 20 professors, 18 assistant professors and 9 CNRS researchers.

INPT was a member of the Scientific and Technical Committee, a major technical contributor in the Conceptual and Numerical work packages (principal author of the SMST interface), and a reviewer in other activities. INPT contributed to Methods and Tools and to the Documentation activities, and delivered a tearing and partitioning component for the CORBA demonstrator.

ASPENTECH

Aspen Technology is a leading supplier of software and services for the analysis, design and automation of process manufacturing plants in industries such as chemical, petroleum, pharmaceuticals, electric power, pulp and paper, and metals.

Aspentech operated in the project through its UK office.

Aspentech was a member of the Scientific and Technical Committee, of the Methods and Tools group, and a major technical contributor in the Conceptual, Thermodynamics/Physical Properties and Unit Operations work packages. Aspentech was the principal author of the Thermodynamics and Physical Properties interface, and delivered several software components for the COM demonstrator.

HYPROTECH

Hyprotech Europe is the European Division of Hyprotech, one of the companies of the UK-based holding AEA Technology. AEA Technology has 4200 employees world-wide, 2400 of which have technical/engineering training. Hyprotech is the main company in the Engineering Software Division.

Hyprotech was a member of the Scientific and Technical Committee, of the Methods and Tools group, and a major technical contributor in the Conceptual, Unit Operations and Thermodynamics/Physical Properties work packages. Hyprotech was the principal author of the Unit Operations interface, and delivered several software components for the COM demonstrator.

SIMSCI

SimSci is a leading provider of commercial simulation software and related services to the petroleum, petrochemical, and industrial chemical process industries as well as the engineering and construction firms that support those industries.

SimSci operated in the project through its UK office.

SimSci was a member of the Scientific and Technical Committee, of the Methods and Tools group and a technical contributor in several areas. Because of internal restructuring, SimSci’s role in the project decreased from being a full member to acting only as a consultative partner. Therefore SimSci did not contribute any software prototype for the project.

QUANTISCI

QuantiSci Limited was formed in 1987 and is a scientific software and consulting company. It specialises in software development and engineering, mathematical modelling, simulation and process engineering. QuantiSci Limited employs around 65 people in offices situated in Henley-on-Thames & Melton Mowbray (UK), Denver (USA) and Barcelona (Spain).

QuantiSci was a member of the Scientific and Technical Committee, of the Methods and Tools group and a technical contributor in all areas. QuantiSci was the « neutral » advisor on software and process simulation technologies. QuantiSci’s major technical contribution were on conceptual issues, requirements analysis, software development process, validation strategies. QuantiSci delivered test harnesses for testing the interface specifications, and was the main author of numerous documents throughout the project.

4. Technical Achievements[1]

The ever increasing usage of mathematical models in all aspects of process development, design and operation has been well documented in several recent studies. This increase in demand is matched by a significant increase in the supply of increasingly sophisticated modelling software from a variety of sources including process engineering software companies, automation system vendors and academic institutions as well as in-house developments within operating companies.

Some of the above software is intended to carry out a narrow, well-defined function such as the computation of physical properties, the simulation of a particular unit operation, or the numerical solution of certain types of mathematical problems arising in process simulation or optimisation. On the other hand, other software tools are essentially environments that support the construction of a process model either from first-principles or from libraries of existing models, or both. They then allow the user to perform a variety of different tasks, such as process simulation or optimisation, using this single model of the process. To achieve their latter function, the second category of process tools incorporate or make use of several software tools of the first category. The distinction between these two kinds of software, albeit in practice not always as clear as described above, is particularly important for the purposes of this report. We shall call them Process Modelling Components (PMCs) and Process Modelling Environments (PMEs) respectively.

The CAPE-OPEN project started in January 1997 and was concluded in June 1999. Its main aims have included the following:

- the identification of major classes of PMCs and the formal definition of general interface(s) for each class;
- the construction and testing of appropriate prototype software demonstrating the use of the above interfaces and the benefits that may arise from it;
- the dissemination of the results of the project leading to the understanding, acceptance and adoption of open software architectures by the process engineering community.

4.1 Scope of the CAPE-OPEN Project

Open architectures can be beneficial for many different types of process engineering software. The specific focus of the CAPE-OPEN project has been on general tools for process modelling and, in particular, their use for steady-state and dynamic simulation. Moreover, the project has recognised

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[1] This section uses excerpts from [Braunschweig B. et al] Open Software Architectures for Process Modelling: Current Status and Future Perspectives, FOCAPD'99 Conference, under permission from the conference organisers.

explicitly the de facto existence and widespread practical usage of two different types of such tools, namely the "modular" and "equation-orientated" ones .

In order to identify the key classes of PMCs that a standardisation effort, such as CAPE-OPEN, needs to address, it is instructive to consider "typical" architectures for process modelling tools. A common, albeit somewhat simplified, architecture for modular tools is shown in Fig.1 below.

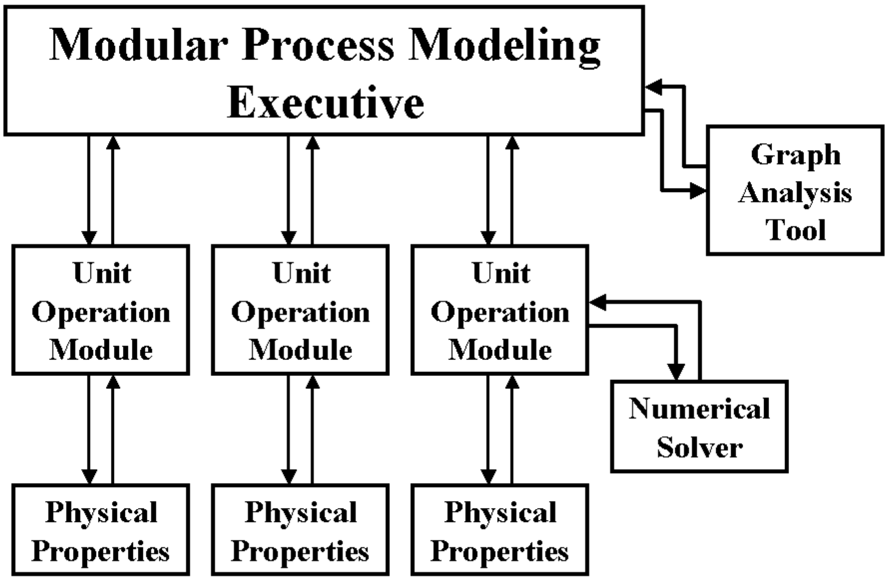


Figure 1: Typical architecture for modular process modelling tools

As shown in the above figure, overall responsibility for constructing a model of a process and carrying out various computations with it is vested in a "process modelling executive". The latter interacts with modules describing individual unit operations. Typically, these will need to interact with packages used to compute the physical properties that occur within the unit operation models. As has already been mentioned, in the modular case each unit operation module will also need to solve the equations of the corresponding mathematical model; the solution may be performed by specialised algorithms (often coded within the unit operation modules themselves), or by making use of external numerical solvers (as shown in the case of the third unit operation module in Fig. 1).

An important characteristic of modular process modelling tools is the need for the executive to organise and co-ordinate the computations carried out by the individual unit operation modules. This often involves the analysis of the process flowsheet to identify "partitions" that may be solved independently, or sets of streams that have to be "torn" to remove cyclic dependencies (see Westerberg et al., 1979). Appropriate flowsheet analysis tools, usually based on graph-theoretical concepts, are used for this purpose.

A typical architecture for an equation-orientated package is shown in Fig. 2. Although the basic structure is not too different from that shown in Fig. 1, a fundamental difference is that the unit operation modules no longer have responsibility for solving their own equations. Instead, they pass information on them to the executive which assembles them into a (typically large) set of equations which it then solves by interacting with one or more appropriate numerical solvers.

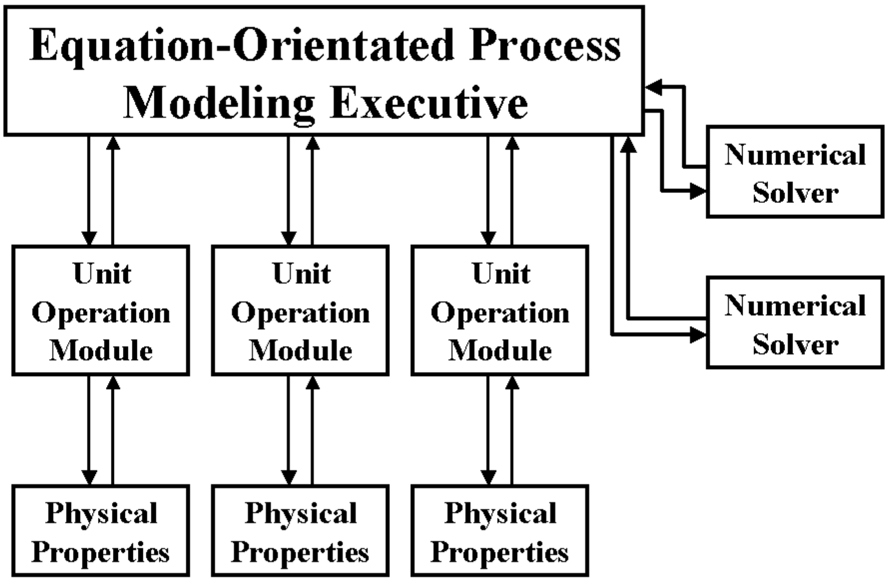


Figure 2: Typical architecture for equation-orientated process modelling tools

The above analysis leads naturally to the identification of the following important classes of PMCs that are prime candidates for standardisation:

- Physical properties
- Unit operation modules
- Numerical solvers
- Flowsheet analysis tools.

Moreover, the analysis suggests that the unit operation modules class has to be sub-divided into two distinct sub-classes exhibiting different behaviours, corresponding to use within modular and equation-orientated packages respectively. The different behaviours may be combined in a single module—so called “dual-mode” models.

The ultimate vision of CAPE-OPEN is to allow complex process modelling tasks and model-based applications to be performed successfully and cost-effectively via the collaborative use of software components coming from a wide variety of sources and possibly being executed on different computer hardware. An example of this is shown in Fig. 3. Here, the PME (the simulator executive and the user interface) is supplied by one vendor, whereas the PMCs (e.g. one or more unit operations, the physical properties calculations, the solution algorithm) come from different suppliers. Extending this principle, the individual components will be able to communicate in a standard fashion with other environments such as process control and monitoring systems, or costing applications.

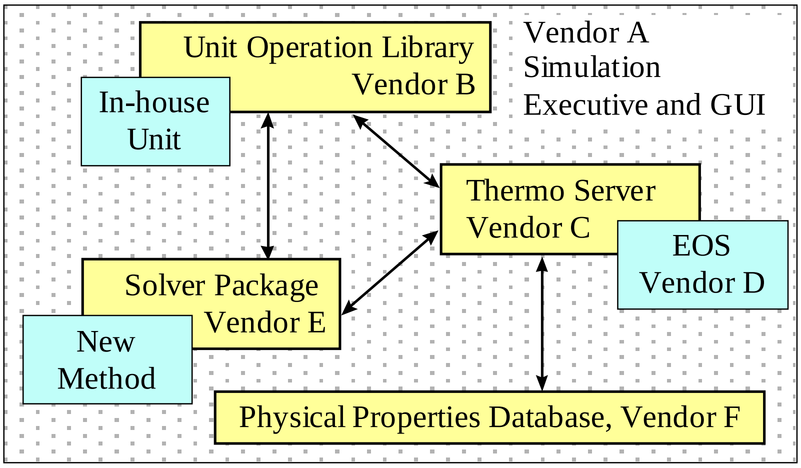


Figure 3: Vision of a typical CAPE-OPEN modelling tool

4.2 PMC Interfaces Defined by CAPE-OPEN

The previous section has identified some of the key classes of PMCs that are prime candidates for standardisation. In view of the very wide range of materials and unit operations employed by the process industries as well as the range of solution techniques used for dealing with different model-based applications, it is not surprising that each of these PMC types can be sub-divided further into several more sub-classes. Clearly, not all of these can be handled within a project of limited duration and resource. This section considers in greater detail the actual scope of each type of interface defined by the CAPE-OPEN project. It also describes the key concepts underpinning each interface and its main characteristics.

For each interface, the corresponding major deliverables are (i) the “Open Interface Specifications Document (public); (ii) the Open Interface Software Prototypes (access restricted); (iii) in some cases, test harnesses and workbench prototypes (restricted).

4.2.1 CAPE-OPEN Physical Property Interfaces

In the area of physical properties, CAPE-OPEN has focused on uniform fluids that are mixtures of pure components or pseudo-components, and whose quality can be described in terms of molar composition. The physical properties methods that have been provided with standardised interfaces are those required for the calculation of vapour-liquid-liquid-solid equilibria or subsets thereof, as well as other commonly used thermodynamic and transport properties.

A key concept in CAPE-OPEN is that of a Material Object. Typically, each distinct material appearing in a process will be characterised by one such object.

Each unit operation module may interact with one or more material objects. For instance, a module modelling the separation of an input stream into vapour and liquid output streams using a non-equilibrium model may interact with 4 Material Objects, representing the material in the input and output streams as well as at the vapour-liquid interface respectively. This interaction may take a number of different forms including setting the values of the Material Object's independent ("state") variables, asking the object to compute a set of pure component or mixture properties for one or more phases at the current values of the state variables or to carry out phase equilibrium calculations, and requesting the current values of some of these properties. Partial derivatives of physical properties with respect to the independent variables can also be computed.

In practice, Material Objects will compute physical properties or perform phase equilibrium calculations by reference to thermodynamic property packages which, in turn, carry out these tasks by making use of thermodynamic property calculation routines and equilibrium servers.

In order to support the implementation of the above framework, CAPE-OPEN has defined standard interfaces for Material Objects as well as thermodynamic property packages, calculation routines and equilibrium servers. The design of all these interfaces has paid particular attention to important issues such as extendibility and efficiency. For instance, the list of properties that any thermodynamic property package is capable of computing is not fixed but can be obtained by client software via a method provided by the corresponding object. Moreover, the interfaces support "batching" of the computation of two or more properties, thereby permitting the exploitation of any common computations shared by these properties.

4.2.2 CAPE-OPEN Unit Operation Module Interfaces

CAPE-OPEN has defined a comprehensive set of standard interfaces for unit operation modules being used within modular PMEs. We review some of the key concepts underpinning these interfaces below.

A unit operation module may have a number of ports which allow it to be connected to other modules and to exchange material, energy or information with them. In the material case (which is also the most common), the port will be associated with a Material Object (see above). Ports also have directions (input, output, or input-output).

Unit operation modules also have sets of parameters. These represent information which is not associated with the ports but which, nevertheless, the modules wish to expose to their clients. Typical examples include equipment design parameters (e.g. the geometry of a reactor) and important quantities computed by the module (e.g. the capital and operating cost of a reactor).

A unit operation module may have its own user interface that allows the user to configure each instance of this module in an appropriate fashion. Typically this configuration will take place at the time when the instance is inserted in a flowsheet and may involve a specification of the precise mode of operation of the unit and the provision of values for the associated degrees of freedom.

Finally, a unit operation module may be capable of producing one or more reports on the results of its computations. Other facilities include the ability of a unit to perform (potentially complex) initialisation computations, to save its current state and to restore it at a subsequent point in time.

The unit operation interfaces defined by CAPE-OPEN allow PMEs and other clients to take advantage of the flexibility afforded by the above features. The computation of a unit operation module is triggered explicitly by its clients via the invocation of a method provided by the unit operation object.

Much of the above considerations also apply to equation-orientated unit operation objects. A key difference is that, instead of carrying out any computations, the main responsibility of the object is to form and expose a set of mathematical equations. Typically, an equation-orientated PME will assemble the sets of equations from the various units in the process into one large set; it will extend this set with equations reflecting unit connectivity and, potentially, other specifications; and it will solve the resulting square system of equations to produce the solution. A key prerequisite for this mode of operation to be feasible is the introduction of formal ways of specifying sets of equations of various kinds. This problem has also been addressed by CAPE-OPEN in the manner described below.

4.2.3 CAPE-OPEN Numerical Solver Interfaces

In the area of numerical solvers, CAPE-OPEN has focused on the solution algorithms that are necessary for carrying out steady-state and dynamic simulation of lumped systems. In particular, this includes algorithms for the solution of large, sparse systems of non-linear algebraic equations (NLAEs) and mixed (ordinary) differential and algebraic equations (DAEs). Algorithms for the solution of the large sparse systems of linear algebraic equations (LAEs) that often arise as sub-problems in the solution of NLAEs and DAEs have also been considered.

A technical difficulty encountered in this context is the large amount of information that is necessary for the definition of a system of non-linear equations. In fact, this amount increases as more and more sophisticated solution algorithms are being developed. For instance, most modern codes for the solution of large DAE systems require information on the scarcity structure of the system, as well as the ability to compute both the residuals and the partial derivatives of the equations. Even more sophisticated codes need further information on any discontinuities that may occur in the DAE system, the logical conditions that trigger these discontinuities and so on.

To overcome the above problem in a systematic manner, CAPE-OPEN has introduced new concepts, such as Models and the Equation Set Object (ESO) which is a software abstraction of a set of non-linear algebraic or mixed (ordinary) differential and algebraic equations. The standard ESO interface allows access to the structure of the system (i.e. the number of variables and equations in it, and its scarcity pattern), as well as to information on the variables involved (i.e. their names, current values and lower and upper bounds). It also allows the ESO's clients to modify the current values of the variables and their time derivatives, and to request the corresponding values of the residuals and partial derivatives (Jacobian matrix) of a subset or all of the equations in the system.

The equations in any Model may involve discontinuities (e.g. arising from transitions of flow regime from laminar to turbulent and vice versa, appearance and/or disappearance of thermodynamic phases, equipment failure and so on). Discontinuous equations in a Models are represented as State-Transition Networks (STN). At any particular time, the system is assumed to be in one of the states in the STN and its transient behaviour is described by a set of DAEs which is itself an ESO. Transitions from one state to another occur when defined logical conditions become true; the Model interface provides complete access to the structure of these logical conditions as well as allowing their evaluation. Such information is essential for the implementation of state-of-the-art algorithms for handling of discontinuities in dynamic simulation.

Any CAPE-OPEN compliant code for the solution of systems of NLAEs or DAEs provides a “system factory” interface. Typically, client software starts by creating a Model that contains a complete mathematical description of the problem being solved. It then passes this Model to the appropriate system factory to create a “system” object that combines an instance of the solver with the Model to which the solver will be applied. The system object then provides appropriate methods for solving the problem completely (in the case of an NLAE system) or advancing the solution over time (in the case of DAEs).

As explained above, the primary aim of the introduction of the ESO and Model concepts is to support the operation of CAPE-OPEN compliant non-linear solvers. However, an important side benefit is that it also provides a general mechanism for PMEs to expose the mathematical structure of models defined within these PMEs. Thus, it may fulfil the role of “model servers” providing the basis for the development of new types of model-based applications beyond those that are supported by the PMEs themselves.

4.2.4 CAPE-OPEN Specific Sequential Modular Tools Interfaces

A key part of the operation of sequential modular simulation systems is the analysis of the process flowsheet in order to determine a suitable calculation sequence for the unit operation modules (cf. Fig. 1). Thus, typically the set of units in the flowsheet is partitioned into one or more disjoint subsets (maximal cyclic networks, MCNs) which may then be solved in sequence rather than simultaneously ("ordering"). The units within each MCN are linked with one or more recycle loops which can be converged in an iterative manner via the identification of appropriate "tear streams" which allow the unit operation calculations to be sequenced.

The above tasks are typically carried out using a set of tools that operate on the directed graph representation of the flowsheet. CAPE-OPEN has defined standard interfaces for the construction of these directed graphs, and for carrying out partitioning, ordering, tearing and sequencing operations on them.

4.3 CAPE-OPEN Implementation and Work Methodology

This section considers some of the issues involved in the implementation of CAPE-OPEN interfaces, and the work process itself adopted by the CAPE-OPEN project.

4.3.1 The Use of Middleware by CAPE-OPEN

The interfaces described in the previous section could, in principle, be implemented in a number of different ways including, for instance, as simple "subroutine" or "procedure" calls in standard procedural languages such as FORTRAN or C. However, CAPE-OPEN has chosen to adopt a component software and object-orientated approach which views each PMC as a separate object. All communication between objects is handled by "middleware" such as the Object Management Group's (OMG) CORBA (Object Management Group, 1997) and Microsoft's COM . These technologies provide standard mechanisms for one software object to interact with another based on a formal interface definition expressed in standard languages also provided by them. The communicating objects can be running as part of the same process, or in different processes on the same or different computer hardware connected in a network, thus providing "local/remote transparency". Issues such as differences in the computer languages in which the various objects are actually implemented, or in the representation of fundamental data types (e.g. real numbers) between different machines are handled automatically. All of these aspects are particularly important in view of the primary aim of CAPE-OPEN to support the interaction of process modelling software components from heterogeneous sources.

Almost all CAPE-OPEN interfaces have been expressed in both CORBA and COM in order to be applicable to a wide variety of hardware platforms and operating systems, and to ensure that they are as “future-proof” as possible in a rapidly evolving environment.

Each CAPE-OPEN interface involves lists of interfaces, methods and arguments expressed in the CORBA IDL and the COM MIDL Interface Definition Languages. Developers of CAPE-OPEN compliant components will need to incorporate the same declarations in their applications and to use IDL compilers of either or both kinds to generate the corresponding instructions in source language such as C, C++, Java, Smalltalk etc. The “wrapping code” generated in this manner can then be linked with the rest of the component. Legacy code, such as FORTRAN models, can also be used by encapsulation within CAPE-OPEN compliant wrappers.

As an example, Fig. 4 shows the simple standard interface specification for accessing some of the ports of a Unit Operation. The method belongs to the ICAPEUNIT interface, takes as input the type and directions of ports required, and returns a pointer to a portsInterface which can then be used to communicate with the selected ports .

INTERFACE NAME		**ICAPEUNIT**
Method Name		GetPorts
Returns		CapeError
Return an interface to a collection containing a list of ports on the unit of a specific type and direction e.g. all input material ports.		
Arguments		
Name	**Type**	**Description**
[in] streamType	CapeStreamType	the type of stream required: material, energy, information
[in] direction	CapeDirection	the direction of flow: input, output or any
[return] portsInterface	CapeInterface	a reference to the interface on the collection containing the specified ports

Figure 4: Typical specification of a CAPE-OPEN method

4.3.2 The CAPE-OPEN Work Process

The definition of interfaces throughout the project was done following a development process based on the UML object-orientated notation for all formal models of the interfaces, including the user requirements, producing use cases, sequence diagrams, state transition diagrams, class diagrams and, finally, interface diagrams which accompany the corresponding middleware implementation (see Table 1). In practice, an iterative approach where the different models and implementations were subject to progressive refinements had to be adopted. Overall, this work process proved to be both an efficient and an effective mechanism for developing commonly agreed standard interface specifications and prototypes meeting those specifications, in a project involving a relatively large number of people with widely different backgrounds.

Phase	Step	Goal
ANALYSIS	User requirements, text	Requirements in textual format
ANALYSIS	User requirements, Use Cases	Use Case models
DESIGN	Design Models	Sequence, state transition, and interface models using UML
DESIGN	UML Repository	UML models in project repository
SPECS	CAPE-OPEN/COM Specification	Draft interface specifications in Microsoft IDL
SPECS	CAPE-OPEN/CORBA Specification	Draft interface specifications in CORBA's IDL
IMPLEMENT	CAPE-OPEN/COM Implementation	Prototype MIDL implementation
IMPLEMENT	CO/CORBA Implementation	Prototype IDL implementation
VALIDATION	Standalone Testing	Tested component
VALIDATION	Integration testing	Tested specification
SPECS	CAPE-OPEN/COM final specifications	Approved specification
SPECS	CAPE-OPEN/CORBA final specifications	Approved specification

Table 1. The CAPE-OPEN development process

4.3.3 Full list of CAPE-OPEN deliverables (documents)

All deliverable documents are public-domain and can be found on the Global CAPE-OPEN web site.

The URL at the time of writing is http://www.quantisci.co.uk/CAPE-OPEN. The web server will be transferred to RWTH Aachen. Its URL will be http://Sunsite.Informatik.rwth-aachen.de/CAPE-OPEN or www.cape-open.org.

CO ROADMAP
CONCEPTUAL DESIGN DOCUMENT ("CDD2")
CO CONCEPTS DOCUMENT
CO OPEN INTERFACE SPECIFICATIONS: THERMODYNAMIC AND PHYSICAL PROPERTIES
CO OPEN INTERFACE SPECIFICATIONS: UNIT OPERATIONS
CO OPEN INTERFACE SPECIFICATIONS: NUMERICAL SOLVERS
CO OPEN INTERFACE SPECIFICATIONS: SEQUENTIAL MODULAR SPECIFIC TOOLS
CO SIMULATOR EXECUTIVE
CO VALIDATION REPORT
CO PATH REPORT
CO GLOSSARY

5. Exploitation plans and follow-up actions

CAPE-OPEN (CO) provides the foundation for a far broader range of modelling system functionality. This system will not only create unprecedented flexibility for achieving major improvement and rationalisation with existing simulation tools, but will also expand the areas of simulation applications by an order of magnitude or more. It is predicted that it will dramatically increase the benefit-to-cost ratio for specialised, in-house software including legacy systems that represent investments of hundreds of man-years of proprietary engineering know-how. At the same time, availability of simulation platforms and frameworks with standard interfaces will make it possible for new application developers to create new value adding software without costly duplication of generalised capabilities, such as physical properties and thermodynamic behaviour.

5.1 Value

Estimating value may be approached by different methods. One approach is to extrapolate results of empirical case studies across the industry. An alternative approach is to build value models based on more detailed and fundamental analysis. Both approaches are used. The latter method tends to be done within major manufacturing companies in order to evaluate decisions on internal resourcing of modelling activities. One CAPE OPEN partner estimates potential annual benefits for modelling and simulation to be in the area of 100 mECU within its own operations.

Case studies of modelling and simulation software indicate that more effective use of modelling and simulation can achieve investment productivity gains of the order of 10-40% of initial plant investment, with operating benefits in the area of 5-20% of manufacturing cost. When applied to European industry, this is consistent with previous estimates of potential capital expenditures savings of more than 400 mECU per year, and operating cost reductions in excess of 300 mECU per year. Corollary benefits are predicted for software maintenance and training costs, which will be reduced substantially as a result of more consistent simulation tools that conform to common standards. A further competitive benefit will be that the crucial time to market is reduced for new innovative products and for processes used to make these products.

Supporting major value is a strongly held conviction by European industry leaders and managers. Their perception is that more value will come from two areas. The first area will be moving from an information or data focus to an understanding or model-based focus of what are complex processes. The second area of benefit will come from changing the way process engineering is done and the way plants are maintained and operated. The conviction is that combining better process understanding with better work practices will lead to achieving several-fold reductions in cycle time and substantial improvement in capital productivity. CO paves the way for these advances in process understanding and work practices.

We can anticipate that if the market settles down, the following behaviour by major manufacturers can be expected.

They will increasingly rely on service providers and integrators who will package key parts of simulation technology and provide them as solutions. This has to happen as an inevitable result of the demographics of these companies and because of new strategies for success that have been defined by these companies.

They will expect that solution providers will provide products that are standard, or at least standards based. One of the goals is to escape from a dependency on legacy or proprietary technology that is an expensive inefficient duplication of work that does not produce competitive advantage. Not demanding standards would result in a worse situation in terms of system vulnerability.

They will expect that solution providers will address the horizontal systems integration area for them, because this area is becoming more and more difficult for companies to address by themselves. These systems will encompass the enterprise and they will be global. They will encompass E Commerce, and they will be impacted in a major way by the enormous changes that result from the explosion of Web and Internet technology.

The implications of this market assessment for exploitation are clear. In particular, we must

- Continue the thrust towards standards.
- Provide the basic infrastructure that are required by standards activity.
- Anticipate and facilitate the major reallocation of key technology skills among organisations within the industry. We need to welcome and embrace change, even if it causes initial discomfort as a result of tradition, rather than some real market or technical factor. We should expect to create and nourish new relationships as part of the shift in the balance of technology to new specialised organisations that exemplify the service and solutions approach, as contrasted with a product approach. CO standard and other complementary standards are what make all of this possible.
- Engage in a dialog with other standards activities. This includes the logical complementary work by groups such as pdXi, STEP etc, but is also needs to encompass the enterprise computing area.

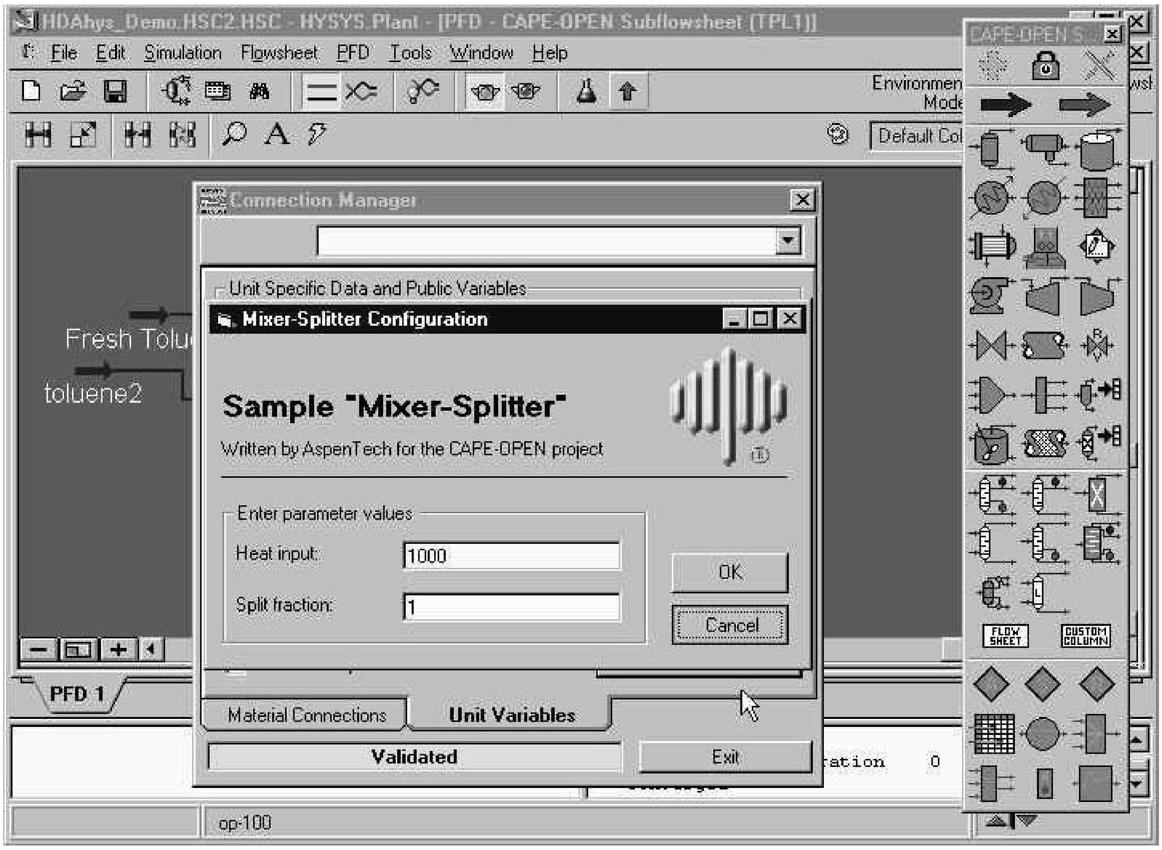
5.2 Industrial and Intellectual Property Rights

There is no plan to patent results of work done in CAPE OPEN. This reflects the fact that the project is directed towards the development of standards that will be promoted world-wide. This in turn reflects the fact that the largest suppliers of current modelling and simulation software sell their products into a world-wide market. In fact, the world-wide industry has expressed general support for CAPE OPEN and there is an expectation that the standards developed will be adapted as «de facto» world standards.

None the less, there will be important advantages. These include the fact that leading European companies have the opportunity to ensure that the standards satisfy their needs, and these same companies will have a significant lead time in working to integrate internal software with the developing standards.

The CAPE-OPEN Exploitation Plan has to be understood in the context of the wider Global CAPE-OPEN Exploitation Plan. In fact, Global CAPE-OPEN presents itself as the first step in practically exploiting CAPE-OPEN results. A specific WP in Global CAPE-OPEN exists with the purpose of developing the first set of CAPE-OPEN components based in existing in-house operating companies' legacy code. In addition Global CAPE-OPEN's CO-LaN will represent the bridge through which CO and GCO results will find their place in the simulation market.

6. Results and Conclusions



HDAhys_Demo.HSC2.HSC - HYSYS.Plant - [PFD - CAPE-OPEN Subflowsheet (TPL1)]

Connection Manager

Unit Specific Data and Public Variables

Mixer-Splitter Configuration

Sample "Mixer-Splitter"

Written by AspenTech for the CAPE-OPEN project

Enter parameter values

Heat input: 1000

Split fraction: 1

Validated

op-100

Figure 5: Aspentech Unit Operation running inside a Hyprotech Simulator Executive

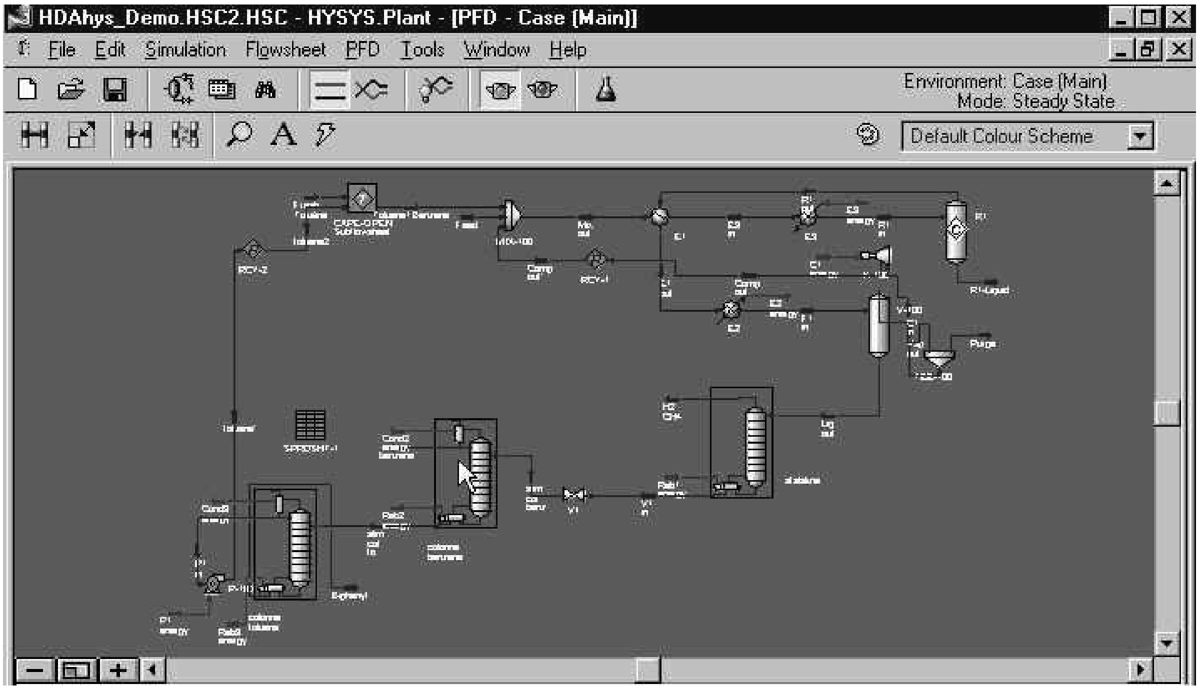


Figure 6: The converged hydrodealkylation of toluene process

6.1 Major accomplishments

The first major accomplishment of CAPE-OPEN was to bring the major players in the process simulation business – representative operating companies, market-leading software vendors, and leading research institutes – to the same table, in order to reach agreement on requirements, priorities, conceptual and even technical standard definitions in a relatively short time. There are now initial agreed specifications for all major areas of process simulation, i.e. unit models, thermodynamics, numerics.

The second accomplishment was the development and evaluation of a large set of methods and tools which were a necessary prerequisite to enable this Europe-wide process with acceptable costs. The choice of innovative component-oriented interface standards has been a critical success factor, even though its implementation was made difficult by the ongoing competition between OMG's CORBA standard and Microsoft's COM standard. In the end, standards were developed in both COM and CORBA, linked by a more abstract specification based on the Unified Modelling Language (UML) and a set of jointly agreed use cases.

6.2 The CAPE-OPEN Demonstrations

The feasibility and industrial potential of the CAPE-OPEN standard is illustrated by two demonstrations, the COM developed by the simulation software vendors Aspentech and AEA-

Hyprotech to show short-term exploitation potential, the CORBA demo by RWTH Aachen to illustrate a path into the future of heterogeneous simulation environments.

The COM demonstration shows exchange of components between the products of two of the market-leading vendors, building on the CAPE-OPEN standards for Unit Models and Thermodynamics. This demonstration, using Microsoft's Component Object Model (COM) as a basis, illustrates the commitment of vendors to enable, in the short range, the operating companies to combine the best partial solutions from both vendors without costly work-arounds.

The CORBA demonstration shows interoperability across a wide range of commercial and research tools on a fully heterogeneous network of different computing platforms and different operating systems, developed independently in several European countries. Specifically, the prototype includes (i)French-developed commercial unit models from IFP, (ii) the English gPROMS numerics system from Imperial College, and (iii) the IK-CAPE thermodynamics package of the German chemical industries. In addition, several new units exploiting this base combination were implemented, including a simple CORBA-based integration workbench from RWTH Aachen and a graph analysis tool from the French Institut National Polytechnique de Toulouse. This demonstration impressively demonstrates that CAPE-OPEN has reached its triple goal of helping to open the simulation market for niche vendors of specialised components, to enable new solution combinations to address novel simulation issues in the process industries, and to foster co-operation on process simulation within Europe.

6.3 Summary and Outlook to Global CAPE-OPEN

Summarising, CAPE-OPEN has fully reached its technical goals of understanding and prototyping the techniques required for open simulation environments in the process industries, and of defining a broad range of actual standard interfaces within this framework. It has also reached the possibly more difficult political goal to get the players to talk to each other in order to create a win-win situation between vendors and users. For the subsequent Global CAPE-OPEN project, this leaves the following key objectives:

- To consolidate the CAPE-OPEN results by setting up a management environment for the standard itself, and for the certification and application of compliant components (make the CAPE-OPEN product available)
- To mature the compliant environments to a degree that a number of reference success stories in real process engineering tasks can be created as a basis for the world-wide adoption of the standards
- To explore the broader context of process simulation in order to ensure coherence of CAPE-OPEN with other process engineering standards

- To ensure that CAPE-OPEN is future-proof by exploring changes in the user environment (e.g. higher emphasis on batch), in the precision of modelling tools (e.g. sub-unit modelling) and in the technical environment (e.g. Java Beans, XML).

6.4 The way forward

Although much has been achieved by the CAPE-OPEN project, it represents just the beginning of the move of process engineering software towards truly open architectures. The recently started Global CAPE-OPEN project intends to cover the steady state and dynamic modelling of a much wider range of continuous, batch and hybrid processes.

The simulation software provider companies consider CAPE-OPEN as a key aspect within their strategy of product development. Moreover, CAPE-OPEN is not just perceived as a standard for interoperability with third party products but is also envisioned as an architecture for use by software components within the same company.

The adoption of the CAPE-OPEN standards by a large number of specialised software component providers is perceived as a way of extending the use of modelling software, which, in turn, should provide a competitive advantage to end users, Process Modelling Components providers and also Process Modelling Environments providers. From this perspective, CAPE-OPEN is considered as the basis for a successful collaboration between all these parties.

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8. Appendix: List of common acronyms

The Glossary Document of CAPE-OPEN gives complete definitions of most of the terms used in the CAPE-OPEN reports. This short table only list acronyms used in this report.

BSCW	Basic Support for Co-operative Work. A web-enabled software providing shared workspaces.
CAPE	Computer-Aided Process Engineering
CO	CAPE-OPEN
COM	Common Object Model (© Microsoft Corporation)
CORBA	Common Object Request Broker Architecture (© OMG)
COSTC	CAPE-OPEN Scientific and Technical Committee
GCO	Global CAPE-OPEN project
IK-CAPE	Industrielle Kooperation – CAPE, a German consortium of chemical companies
M&T	Methods and Tools
NUMR	Numerical Work Package
OMG	Object Management Group, a non-profit organization defining interoperability standards
OO-CAPE	Object-Oriented CAPE, a study made for the CO partners in 1995
OS-CAPE	Open Standards for CAPE, a consortium gathering the CO partners in 1996
PdXi	Process Data Exchange Institute, an US consortium
PMC	Process Modeling Component
PME	Process Modeling Environment
SMST	Sequential-Modular Specific Tools
STEP	Standard for the Exchange of Product model Data
THRM	Thermodynamic and Physical Properties Work Package
UML	Unified Modelling Language, an OMG standard notation for Object-Oriented software engineering
UNIT	Unit Operations Work Package