Global CAPE-OPEN

Delivering the power of component software
and open standard interfaces
in computer-aided process engineering

Final Report

The GCO Consortium

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2. Executive Publishable summary

Companies in the Process Industries typically employ a collection of software (in-house, commercial, and/or academic) to solve various Computer Aided Process Engineering (CAPE)-related problems. Ideally, it should be possible to 'assemble' the necessary computational tools with the minimum effort. That has not been possible because the market for process simulation has been one of incompatible proprietary products.

The European CAPE-OPEN project (January, 1997 through July, 1999) established a set of process simulation software standards to allow communication between various pieces of software from different sources (software and equipment vendors, universities, and "home grown"). However, much work was needed to fully implement CAPE-Open standards and the GCO project has been the vehicle for accomplishing that goal.

The GCO consortium represented a wide range of users, researchers, and vendors:

- In Europe: IFP (European and International co-ordinator), AspenTech, BASF, BP, DECHEMA, DTU, ELF, AEA Hyprotech, ICI, Imperial College, INPT, Norsk Hydro, NTNU,RWTH.LPT, RWTH.I5, UPC
- In Japan: Mitsubishi Chemical (regional co-ordinator), JGC, Kyoto University, Tokyo Institute of Technology
- In USA: Dow (regional co-ordinator), Air Products, Carnegie-Mellon University, Honeywell Hi-Spec Solutions, Protesoft Corporation, SIMSCI, University of Massachusetts, University of Virginia, and UOP

At its conclusion, the GCO project, the consortium has obtained the following major results:

- Endorsement of the project by the Intelligent Manufacturing Systems initiative;
- European and international collaboration between partners from France, UK, Germany, Spain, Denmark, Norway, USA, Canada, and Japan.
- Release of the CAPE-OPEN 1.0 Standard, including updates to the major interfaces, and new interface standards for complex materials, optimisation, data reconciliation, access to physical properties databases, real time simulation, hybrid systems, and common services.
- Migration of many existing proprietary software components to CAPE-OPEN compliance;
- Full and efficient interoperability of Unit Operation modules, thermodynamic servers and process modelling environments using commercial software from several vendors;
- Additional research results on lifecycle modelling, web-based process engineering, and high granularity process modelling;
- Creation of the CO-LaN, CAPE-OPEN Laboratories Network, an organisation in charge of maintaining and disseminating the standards, and helping to facilitate the development of compliant process modelling components.

For more information, visit our web site: http://www.colan.org

3. Objectives of the project

We start by restating the major objectives of the project, as presented in the GCO Work Plan:

> The major expected result of GCO will be **the global acceptance of CAPE-OPEN as a standard for communication between components in process engineering**, leading to the availability of software components offered by leading vendors, research institutes and specialized suppliers. This will enable the process industries to reach new quality and productivity levels in designing and operating their plants. This will open new markets for suppliers of CAPE components. This is a major breakthrough as compared to the current state-of-the-art which is that of no integration at all.

How does one measure the global acceptance of CAPE-OPEN as a standard for communication between components in process engineering? A first measure is the number of commercial components implementing the standard. Already two major commercial vendors, AspenTech and AEA Hyprotech, introduced CO compliance in their main CAPE environments (Aspen Plus and Hysys). Several software companies - including SMEs, many universities, and a number of industrial users have done the same. The first part of next section lists the ones that we are aware of.

Another measure is the status of CAPE-OPEN within the CAPE community. First, it is important to mention that **Global CAPE-OPEN has been the world-wide initiative for defining interoperability standards for CAPE components**. There are no competing initiatives. We included many of the leading providers, researchers and users of the technology, and all others have been looking at us. The links to our website when searched with Google or other popular search engines show that it is very well referred! CAPE-OPEN and Global CAPE-OPEN have been extensively presented in conferences, publications, vendors meetings, and journals. The AIChE magazine, Chemical Engineering Progress, published a long article on CO and GCO in its September 2000 issue. This magazine has 70,000 subscribers and 100,000 readers at least. The "physical properties" community decided to host a GCO workshop in their triennial meeting in Kurashiki, Japan, May 2001. The ESCAPE-11 conference in Kolding, Denmark, May 2001, hosted a GCO session and a GCO "open room".

This is enough for the strategic aspects. Let us now look at each specific objective, one by one, and assess where we are at the end of the project.

- ***New Open Interface Specifications in other domains and application areas of CAPE ;***

Achieved. New interface specification have been released in the CAPE-OPEN 1.0 standard, including specifications for complex materials, optimisation, data reconciliation, access to physical properties databases, real time simulation, hybrid systems.

- ***Sets of compliant software components developed by the vendors, operating companies and academics involved in GCO ;***

Achieved. As written above, the list of compliant software is presented in the scientific and technical assessment section.

- ***Guidelines on how to integrate process simulation components at the work place, including selection criteria, quality assurance measures and training programs for process engineers ;***

Not fully achieved, but significant progress has been made, see WP4 report.

- ***Software prototypes of additional components which take advantage of the standard interfaces for providing added value;***

Achieved. For all new interfaces, prototypes have been developed and tested in the second half of the project.

- ***Experience in downloading process engineering software components through I-Nets , allowing a new framework for collaborative work in CAPE, independently of geographical and organisational frontiers ;***

Not fully achieved. It has been experienced in WP6.1 through the "web-based simulation" example but there is much more to be done in order to establish web-based collaborative e-CAPE! See WP6 report.

- ***A CAPE-OPEN Laboratories Network, aimed at managing the lifespan of the CO standard by providing guidance to the developers, extending the standard, conducting the compliance tests and certifying submitted components. After the GCO project, the CO-LaN will live on its own through international funding from operating companies, software vendors and academy.***

Achieved. The CO-LaN exists as an organisation since January 2001 and now lives on its own. The Master Plan and Bylaws of CO-LaN are annexed to this report. There are a few differences from the initial master plan (we have learned by doing) but the main goal is still there and the CO-LaN is reaching it.

4. Scientific and Technical assessment

Since the project is organised in eight workpackages, the presentation follows the same structure.

The project uses a shared workspace on the web, based on the BSCW software (Basic Support for Collaborative Work), and hosted by RWTH.I5. When using the term "BSCW", the reports refer to locations within this workspace.

We start with a subsection presenting the CAPE-OPEN 1.0 standard, one major result of the GCO project. This is taken from Volume 2 of CAPE-OPEN Update, a newlsetter produced by the GCO-Support project, an accompanying measure for GCO, funded by the Competitive and Sustainable Growth Programme, and distributed by the CO-LaN.

4.1 The CAPE-OPEN 1.0 Standard

The CAPE-OPEN 1.0 standard, a product of several years of collaborative work between partners and contractors of the CAPE-OPEN and Global CAPE-OPEN projects has been recently released and is available for download from the www.colan.org CO-LaN website.

This article aims at giving an overview of the technical elements of the standard - the set of open standard interface specification documents which describe the main software interfaces that process modelling components and environments must provide in order to be CAPE-OPEN compliant. It must be understood that there is no requirement for a piece of software to implement all interfaces specified by CAPE-OPEN. On the contrary, the interface specifications are organised in such a way that each process modelling component (PMC) or process modelling environment (PME) only needs to implement a limited and focused set of interfaces to allow it to interoperate with other software. As an example, a Unit Operation software component (e.g. a model of a distillation column, of a reactor, of a heat exchanger, or a pump etc.) is only required to implement Unit Operation "plug" interfaces, plus a small number of Common Services interfaces, in order to be used with a CAPE-OPEN compliant PME. Should the Unit Operation require direct use of a Physical Properties or of a Chemical Reactions component for internal calculation, then it would have to implement physical properties or chemical reactions "sockets" interfaces in order to gain access to these services.

Note that we have been using the terms *socket* and *plug* to refer to the calling and called components respectively: where a software component **A** requires service **S** from component **B** through a published CAPE-OPEN interface specification of service **S**, **A** is said to implement an **S** *socket*, and **B** is said to implement an **S** *plug*.

In the following, we will look at the architecture of CAPE-OPEN 1.0 interfaces, we will briefly address performance issues, and we will give a list of currently available implementations of CAPE-OPEN interfaces in both commercial and research PMCs and PMEs. Some of the text is borrowed from J.-P. Belaud and M. Pons, " *Open Software Architecture For Process Simulation: The Current Status of CAPE-OPEN Standard*", to be presented at ESCAPE-12 conference, The Hague, May 2002, with permission from the authors.

Technical elements of CO 1.0

The CAPE-OPEN interfaces are split in three groups corresponding to three blocks of functionality: business interfaces (also called PMC interfaces), COSE interfaces (also called PME interfaces), and common services. They were introduced by J.-P. Belaud in Vol.1 of this newsletter:

- *Business interfaces* or *PMC Interfaces* are domain-specific interfaces for the CAPE application domain. They define services provided by CAPE-OPEN compliant process modelling components involved in a CO modelling application. Examples are Unit Operations, Thermodynamic and Physical Properties, Solvers, Physical Properties Data Bases, etc.

- *COSE (CAPE-OPEN Simulator Executive) Interfaces* or *PME Interfaces* are horizontal interface specifications. They define services provided by CAPE-OPEN compliant PMEs. Services of general use are defined, such as *diagnostics* and *material template system* in order to be called by any CO PMC using a callback pattern.
- *Common Services Interfaces* define services that may be required by any *Business* and *COSE interfaces*. They support basic functions, such as identification, error handling, collections of objects, parameters, etc.

The first set, *business/PMC interfaces*, is a comprehensive set of functionalities of process modelling application elements. Let's look at it in detail.

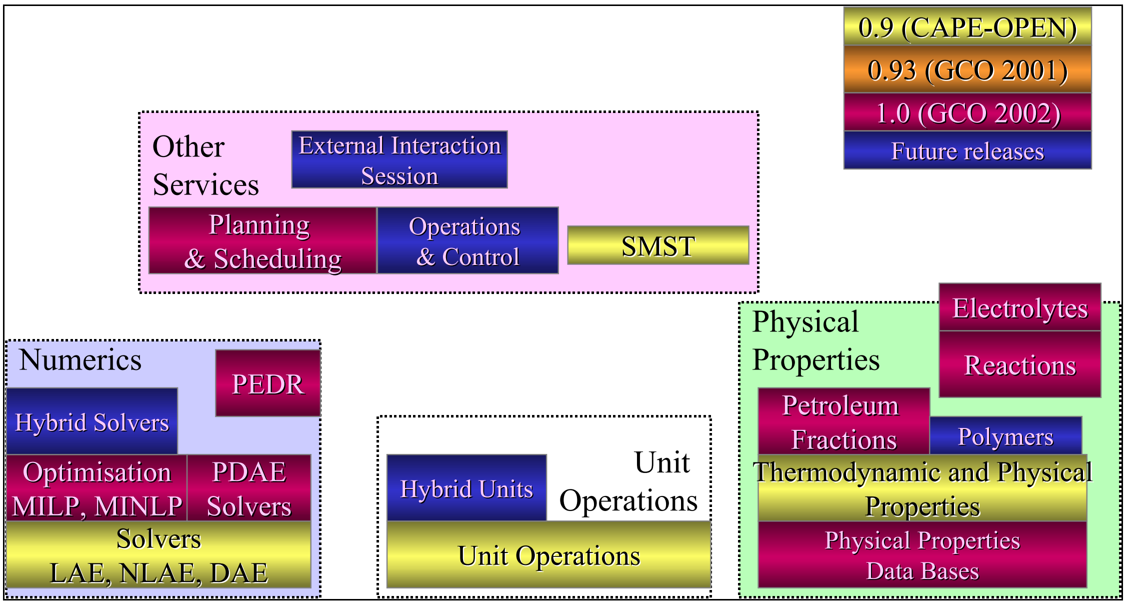

Figure 1: CAPE-OPEN Interfaces for Process Modelling Components

Business interfaces can be roughly grouped in four categories, as shown above: numerics, unit operations, thermodynamic and physical properties, and others. Although it can be debated if chemical reactions/electrolytes interfaces should be kept together with physical properties, we will keep them as such, since is it merely a question of presentation - there are no technical implications.

Version 1.0 updates previously published interfaces (known as "CAPE-OPEN 0.93") and delivers brand new interfaces. These new interfaces have not been as extensively tested as the ones previously published, therefore will be subject to updates after subsequent implementation in operational software. They are identified by the **New!** sign.

Several interfaces have been extensively tested and debugged by the Interoperability Task Force of Global CAPE-OPEN, a group of specialists led by Peter Banks and Malcolm Woodman of BP. They are identified by the **"ITF-ed!"** sign.

The *Numerics* class groups services related to numeric processing of process models.

- The base interface in this class is *Solvers*: it focuses 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 are also considered. The CO standard introduces 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.

- **New!** The *PDAE (Partial Diffential Algebraic Equations)* interface defines, on top of the *Solvers* specification, numerical services for systems with some variables distributed along one or several dimensions. In PDAEs the dependent model variables depend on one or more independent variables. Independent variables are for instance spatial co-ordinates, particulate co-ordinates (in case of population balance models) or time (in case of dynamic models). Thus, models of computational fluid dynamics are also included in this class of problems.
- **New!** The *Optimisation* interfaces define access to Mathematical Programming optimisation services. They are also based on the *Solvers* architecture. Mathematical programming (IP / LP / NLP / MILP / MINLP) problems involve the minimisation or maximisation a linear / nonlinear objective function subject to linear / nonlinear constraints. The optimisation may involve both continuous and discrete (integer-valued) decision variables. Mathematical programing optimisation problems arise in many process engineering applications, including process synthesis, process design, product design and others.
- The *Hybrid Solvers* interface is not part of CAPE-OPEN 1.0 release and is not addressed here.
- **New!** The *Parameter Estimation and Data Reconciliation* interface (PEDR), at its name clearly states, defines interface to (i) parameter estimation algorithms where the value of a model parameter must be adjusted in order to meet constraints such as experimental data; and (ii) data reconciliation packages which eliminate noisy factors from raw measurements of process variables; The DR and PE are very similar problems in the sense that both are constrained optimization problems. Since a PEDR module may require using external optimisation services, the PEDR module may call an optimisation solver module through a CO-compliant interface.

The *Unit Operation* class groups two services related to unit operations.

- **ITF-ed!** Base *Unit Operation* component: CAPE-OPEN defines a comprehensive set of standard interfaces for unit operation modules being used within modular and steady-state PMEs. A unit operation module may have several ports that 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 is associated with a Material Object. Ports are given directions (input, output, or input-output). Unit operation modules also have sets of parameters. These represent information that is not associated with the ports, but that 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).
- *Hybrid Unit Operations* extend the base UO interface towards the processing of batch and hybrid UO's. This interface is not part of CAPE-OPEN 1.0 release and is not addressed here.

The *Physical Properties* class groups services related to obtaining or calculating thermodynamic and physical properties of matter, and to handling chemical reactions.

- **ITF-ed!** *Thermodynamic and Physical Properties* base interface: CAPE-OPEN focuses 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 operations that have been provided with standardised interfaces are those required for the calculation of vapour-liquid or liquid-solid equilibria or subsets thereof, as well as other commonly used thermodynamic and transport properties. A key concept is that of a Material Object. Typically, each distinct material appearing in a process (in streams flowing between unit operations, as well as within individual unit operations) is characterised by one such object. To support the implementation of the above framework, the CO standard defines interfaces for Material Objects, as well as for thermodynamic property packages, calculation routines and equilibrium servers.

- **New!** *Physical Properties Data Bases* (PPDB) interfaces define a CAPE-OPEN compliant standard interface for connecting a data base with recorded physical property values and model parameters to flowsheeting and other engineering programs. This interface deals with measured, correlated or estimated values of physical property data at discrete values of the variables of state (temperature, pressure, composition).
- **New!** *Petroleum Fractions* (PetroFrac) interfaces extend the standard Material Object for use in the modelling of hydrocarbon fluids processed in refining, petrochemicals and offshore production facilities. They supply additional access to petroleum-specific properties (e.g. RON, MON, cetane index, TBP curves, etc.), and allow characterising parameters of the mixtures. They also introduce a small change in the Unit Operation interfaces in order to distinguish Unit Operations handling petroleum fractions from others.
- *Polymers* interfaces extend the base Thermo interface towards the processing of polymers. This interface is not part of CAPE-OPEN 1.0 release and is not addressed here.
- **New!** *Chemical Reactions/Electrolytes* interfaces support the management and processing of kinetic, equilibrium and electrolytes reaction systems in process models. These interfaces support any reaction model, they are clients to formulate reaction equations, and they support reaction model parameter estimation. Initially planned as two different specifications, Chemical Reactions and Electrolytes were finally merged into one consistent set[1].

The *Other Services* class groups various services which do not belong to the three main classes. Only two interfaces are part of CAPE-OPEN 1.0, the others (*Operation and Control* and *External Interaction Session)* are published as drafts, but not officially released. They are not presented here

- *Sequential Modular Specific Tools* (SMST) interface. A key part of the operation of sequential modular simulation systems is the analysis of the process flowsheet in order to determine a suitable sequence of calculation of the unit operation modules. This task is typically carried out using a set of tools that operate on the directed graph representation of the flowsheet. The SMST specification defines standard interfaces for the construction of these directed graphs, and for carrying out partitioning, ordering, tearing and sequencing operations on them.
- **New!** *Planning and Scheduling* interface defines interfaces to components delivering procedures and processes for allocating equipment over time to execute the chemical and physical-processing tasks required for manufacturing chemical products, generally in batches. These interfaces deal with managing requirements, production resources, recipes, planning and scheduling problems and their solutions.

COSE/PME interfaces define general services that can be requested from CAPE-OPEN compliant process modelling environments such as Hyprotech's HYSYS, AspenTech's AspenPlus, PSE's gPROMS, or RSI's INDISS. All these specifications are **New!** in CO 1.0. The COSE/PME interface is a small and simple interface with only half a dozen methods. It might be extended in the future.

[1] At the same time, we publish future draft releases (1.1) of Thermodynamic and Physical Properties, and of Reactions; anyone intending to implement these versions should contact CO-LaN.

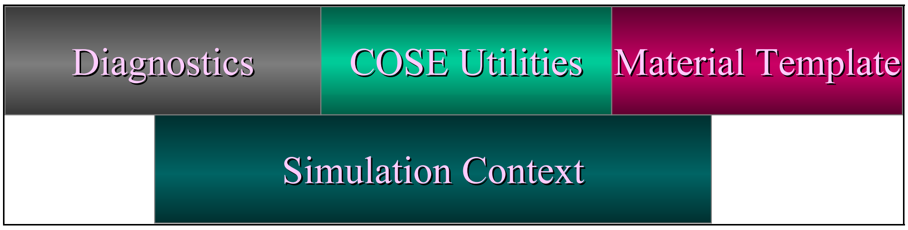

Figure 2: CAPE-OPEN Interfaces for Simulation Executives (or Process Modelling Environments)

- *Simulation Context* interface specification is the base specification for COSE services. It gathers three functionalities, Diagnostic, Material Template System and Utilities. That results in three interfaces, one for conveying verbose information to the PME, one for allowing the unit to choose between all the Thermo Material factories supported by the COSE, and one for requesting diverse values from the PME.
- *Diagnostic* interface allows communication of verbose information from the PMC to the PME (and hence to the user). PMCs should be able to log or display information to the user while executing a flowsheet.
- *Material Template* interface provides the mechanisms for accessing CAPE-OPEN Property Packages managed by the COSE, in order to allow PMCs to directly choose and configure material objects as needed.
- *COSE Utilities* provide a small list of other useful functions, in particular the FORTRAN Channel selection which prevents FORTRAN-based PMCs from sending output to channels already used by the COSE.

Common Services interfaces define base services that CAPE-OPEN components can either use or provide, independently of the nature of the component. Some of these specifications were published in release 0.93 last year, some are new. They are gathered in one of the two "Methods and Tools" documents which were developed by the Methods and Tools group of Global CAPE-OPEN: the Common Interfaces Reference Manual.

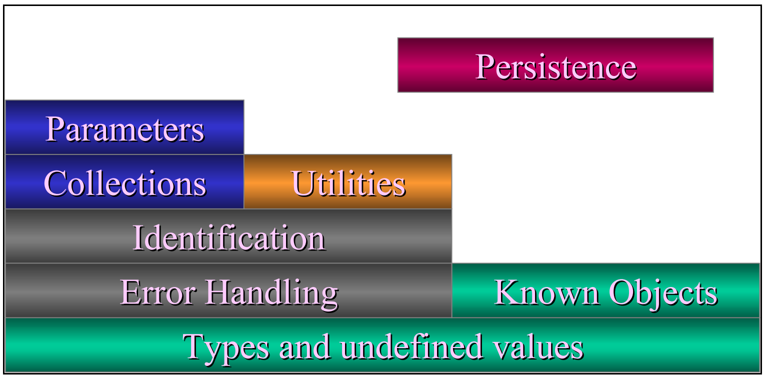

Figure 3: CAPE-OPEN Common Services Interfaces

- **ITF-ed!** *Types and undefined values* are the most basic elements of the CAPE-OPEN 1.0 specification. They define the standard types of all elements passed through CO interfaces: integer values, real values, arrays, character strings, etc. as well as "undefined" values. All CO interfaces rely on the standard types.

- **New!** *Known objects* gather a large number of standard identifiers used in interfaces, such as Thermo, PPDB, and petroleum fractions. These are lists of properties names, names of methods; identification of phases, etc., which form a consistent set of names used throughout these interfaces.
- **ITF-ed!** *Error Handling* defines how to manage execution errors (abnormal terminations). When a request is made, if this request is successful it raises no error, otherwise it raises an error. When an error occurs, the execution is immediately aborted. This *Error Handling* interface gives a classification and a hierarchy of potential errors occurring in CO compliant components. All CO components must implement it.
- **ITF-ed!** *Identification* interface provides the means for all CO components to be identified by name and textual description. All CO components must implement it.
- **New!** *Collections* interface defines a standard way of managing collections of things. The aim of the Collection interface is to give a CO component the possibility to expose a list of objects to any client of the component. The client will not be able to modify the collection, i.e. removing, replacing or adding elements. However, since the client will have access to any CO interface exposed by the items of the collection, it will be able to modify the state of any element.
- **ITF-ed!** *Parameters* interface defines a standard access to component parameters. This specification will be used by CO components wishing to expose some of their internal data to their clients. The interface is made up of two different parts, each corresponding to a different client need: the first part is a fixed, static aspect that describes the Parameter, such as a type, name, description, dimensionality etc. The second part deals with value of the parameter itself. It is expected that the parameter values will change quite frequently both within and outside of the component that needs it.
- **ITF-ed! New!** *Utilities* interface gathers a number of useful functionalities that can be requested from process modelling components. In version 1.0, this interface provides the means to set the simulation context, to collect component parameters, to manage lifecycle of components (creation and termination) and to edit, that is, to open an edit GUI for the component.
- **ITF-ed! New!** *Persistence* interface defines how models and model elements are stored and retrieved. Most simulation environments allow the possibility to store at any moment the state of a simulation case, in order to be able to restore it at any time in the future. In the CAPE-OPEN distributed environment, where different pieces of the simulation may be implemented by different vendors, the Persistence interface proposes a standard mechanism to provide this feature. This interface is different from all others, as it does not define any new method. Instead, it explains how to use standard persistence mechanisms provided by middleware (COM and CORBA) for this purpose.

Performance Issues

The Interoperability Task Force of Global CAPE-OPEN spent considerable effort on performance issues in the last months of 2001. The ITF was charged with facilitating the delivery of practical, plug and play interoperability within commercial flowsheet simulators, via industrially-relevant test scenarios and the critical review of the CAPE-OPEN interface specifications for ambiguities and omissions. This capability within mainstream commercial flowsheet simulators is a prerequisite for acceptance of open simulation in the work place.

Good performance is critical especially for thermodynamic and physical properties calculations which are called thousands of times during a process simulation, so that the overhead due to standard interfaces should be minimal. This issue is also of importance for other components but the focus has been on physical properties and thermodynamics since the initial performance degradation was huge in some implementations.

The result of the ITF work is that there is almost no degradation of performance if the interfaces are correctly and efficiently implemented. Revisions of internal implementation of physical properties components by vendors and others (without any revision of the interface specifications) led to orders of magnitudes of improvement, with final values of around 15-20% overhead in calculation time due to CAPE-OPEN interfaces being possible. Such an overhead is not significant and is very quickly compensated by the consequences of Moore's Law, which makes computing speed higher and higher and computing power cheaper and cheaper.

In conclusion, you should not worry about performance of CAPE-OPEN interfaces in general. You should only worry about efficient implementation of CAPE-OPEN compliant physical properties and thermodynamic services: the development of physical and thermodynamic properties plugs or sockets must take serious care of performance, whether the CAPE-OPEN or any other standard is used.

CO-compliant Process Modelling Components and Process Modelling Environments

The following table lists a number of commercial or research PMCs and PMEs providing CAPE-OPEN interfaces. This table cannot be exhaustive since we cannot be aware of all the current developments and migration of existing software packages to CO compliance. If you are interested in specific software package shown in this list, please contact its supplier. If you are interested in any software package **not shown** in the list, please contact its supplier and ask for CO compliance!

A catalogue of CO-compliant PMCs and PMEs will be published on www.colan.org.

Supplier	Software	Interfaces	Technology
AspenTech www.AspenTech.com	Aspen Plus 11.1	Thermodynamic and physical properties socket, Unit operations socket	COM
AspenTech	Aspen Properties 11.1	Thermodynamic and physical properties plug	COM
Hyprotech www.hyprotech.com	HYSYS.Plant 2.4	Thermodynamic and physical properties socket, Unit operations socket	COM
Hyprotech	Distil	Thermodynamic and physical properties socket	COM
Hyprotech	COMThermo 1.1	Thermodynamic and physical properties plug	COM
Process Systems Enterprise (PSE) www.psenterprise.com	gPROMS	Thermodynamic and physical properties socket, Unit plug	COM CORBA
Process Systems Enterprise (PSE)		Numerical solvers sockets (linear algebraic, nonlinear algebraic, differential-algebraic)	CORBA
Process Systems Enterprise (PSE)	gO:CAPE-OPEN	Equation Set Object (unit) plug	COM
Belsim www.belsim.com	VALI III	Thermodynamic and physical properties socket	COM
Prosim S.A. www.prosim.net	ATOM	Thermodynamic and physical properties plug	COM
Prosim S.A.	Odysseo	Dynamic flash unit plug	COM
Infochem www.infochemuk.com	Multiflash 3.1	Thermodynamic and physical properties plug	COM
RSI www.rsi-France.com	INDISS	Thermodynamic and physical properties plug and socket Unit Operation plug and socket	COM COM
IFP www.ifp.fr	SPIP	Thermodynamic and physical properties plug	
IFP	FIBER	Unit Operation plug	

Supplier	Software	Interfaces	Technology
INP Toulouse-LGC-CNRS www.inp-toulouse.fr/lgc	Numerical Services Provider and Continuous Model Builder M&S	Numerical Solvers plug and socket Unit socket	CORBA COM
INP Toulouse-LGC-CNRS	Flowsheet Server	Sequential Modular Specific Tools plug	CORBA
DECHEMA www.dechema.de	DETHERM	Physical Properties Data Bank Plug	COM
RWTH.LPT www.lfpt.rwth-aachen.de		Numerical solvers plug	CORBA
RWTH.I5 www-i5.informatik.rwth-aachen.de	COM-CORBA Bridge Java Unit Skeleton Java Material Object Skeleton	Bridge Unit Operation plug Material Object and Material Template	COM, CORBA CORBA CORBA
CO-LaN www.colan.org	Tester Suite (1)	Thermodynamic and physical properties plug and socket Unit Operation plug and socket	COM, CORBA through bridging
CO-LaN	Tester Suite (1)	MINLP socket PPDB socket SMST socket & plug	COM
NORSK HYDRO www.hydro.com		Heating Tank Unit Operation Fluent Wrap Unit Operation CASE test socket	CORBA
UPC www.upc.es/eq/	MOPEDR MOPP	PEDR Prototype Planning and Scheduling Package	CORBA CORBA

(1) The CO-LaN tester suite is a comprehensive set of public-domain tools aiming at helping organisations develop CAPE-OPEN components through detailed compliance checking mechanisms. This is one of the methods that CO-LaN uses to facilitate the migration to CAPE-OPEN, together with additional how-to documents (the *migration cookbook*) and software *wizards*.

Conclusion

CAPE-OPEN interfaces match the interoperability needs of the process modelling community; they are debugged; they are efficient; they are publicly available on the web site for anyone to use; they have been implemented in many software packages; in short, they work!

Open process simulation is not a futuristic thing. It is here and now. If you are a supplier, migrate your software to CO compliance; if you are a user, ask for CO compliance from your suppliers.

Acknowledgements

This text summarises many other documents authored by contributors of Global CAPE-OPEN from several organisations. It is better not to give any names, since the list would be too long. Many thanks to all.

In addition, this article was reviewed and commented by Peter Banks, Jean-Pierre Belaud, Kerry Irons, Knut Mathisen, Costas Pantelides, Michel Pons, Luis Puigjaner, and Pascal Roux.

References

The CAPE-OPEN 1.0 standard is downloadable from www.colan.org.

4.2 WP1: Management

4.2.1 Overview of Work

The Management work package had three major responsibilities: managing the project and operating its various committees (task 1.1); defining software methods and tools for the project (task 1.2); supplying communication mechanisms to the partners (task 1.3). The project management and co-ordination aspects are presented in section 7. In this section, we briefly outline some achievements of the work package in terms of management and co-ordination, and of Methods and Tools.

4.2.2 Objectives

Our objectives for the project were:

- To kick off the project and to obtain IMS endorsement on the interregional proposal, as stated in the project workplan;
- To organise the work of the Steering Committee, of the Management Committee, of the Scientific and Technical Committee, of the Exploitation Committee, and more generally of the various groups in the project;
- To define standards, templates, and project guidelines for use by the technical work packages;
- To define and apply an approval process for all documents produced in the project;
- To organise Methods and Tools work and to publish sets of guidelines;
- To train European and International partners to CAPE-OPEN technology;
- To create and operate a web-based collaborative server used by all partners for exchanging project documents and other material;
- To organise the final meeting and prepare the final reports.

4.2.3 Technical progress and Achievements

All objectives listed above have been reached. The project was launched in July 1999. IMS endorsement was obtained in April 2000. All project committees have been active and running throughout the project, with the exception of the Exploitation Committee which was only launched in 2000, and was moved to WP7. Committee activity is presented in section 7 of this report. Standards, templates and guidelines were defined and used by all project partners. The approval process document was defined and applied. The Methods and Tools group has had many meetings, phone conferences, and produced three sets of guidelines. Newcomers were trained in two three-day training sessions. The project BSCW (collaborative work server) operated from July 1999 to March 2002, with a service rate close to 100% (it almost never stopped), and had more than 80 registered users. All project documents are stored on this server. The project final meeting took place in December 2001 in Cambridge, UK, with around fifty attendees.

4.2.4 M&T Achievements

The Methods and Tools group took care of assessing, selecting, adapting and applying software methodologies and tools throughout the project. Basically, the process defined in CAPE-OPEN, which uses the UML notation with a tailored development process, was followed in GCO.

The M&T group provided periodical reports on its work in the form of guidelines documents. At the end of the project, the M&T group's contribution is summarised in the set of " *COSE/PME* interfaces and *Common Services* interfaces that are part of the CAPE-OPEN 1.0 Standard, referenced above.

4.2.5 M&T Work Items

The M&T group worked on the following matters during the project. Most of these correspond to published documents.

- Naming, types and undefined values: a new release of this document was prepared in order to support the latest lists of types and the general usage of undefined values (previously called empty values); it defines how to name interfaces, the basic types for all CO components, and what to do with methods that do not return anything;
- Common services: Error handling: the error handling interface was proposed in October 2000 and was subject to a minor upgrade in June 2001;it defined an error handling mechanism to be used by all CO components;
- Common Services: Parameters: this interface was proposed in October 2000 and revised in March 2001; it defines the use of parameters in all CO interfaces;
- Common Services: Identification: this interface was proposed in October 2000 and did not change since; it defines how components should identify themselves;
- Common Services: Collections : this interface was drafted in February 2001 and revised in May 2001; it defines how CO components should handle collections (sets) of objects;
- Common Services: Edit: this interface was drafted in May 2001; it defines a generic editing facility for all CO components. It is part of the Utilities document.
- Common Services: Persistence: this is not really an interface specification but rather a set of guidelines on how to use persistence (save and restore) mechanisms provided by COM and CORBA; it was published in its final form in October 2001;
- Common Services: Report: this is part of the Utilities document;
- Common Services : Events: the M&T group produced a requirements document on Events, which can form the basis for further development of a generic event handling interface aimed at managing interruptions in calculations, such as pausing and resuming.
- Common Services: Units of Measurement: the M&T group produced an analysis of existing UOM services (i.e. in OpenSpirit) and decided to give a low priority to such a unit conversion service, because all CO interfaces are supposed to work with SI units of measurements;
- COSE Interface: this interface, initially called "Simulation Context Interface", was drafted in March 2001; it defines an access to COSEs (simulator executive) services for all CO components;
- COM and CORBA architectures: two architectural documents presenting the general usage of CO components in COM and CORBA were produced in October 2000 and not revised since that date;
- Link with other project activities: wizards, COM-CORBA bridge, CO tester. These technical developments from WP4 and WP8 were discussed during M&T meetings, a few improvements came out of these discussions.

4.3 WP2: Open Interface Standards for new Modules

4.3.1 Overview of work

This work package addresses the standardisation of open interfaces for a number of important simulation modules and functionalities that were not covered by the earlier CAPE-OPEN project. These includes additional standards physical properties of complex materials, kinetic phenomena, optimisation (including parameter estimation and data reconciliation), distributed information and future standards.

Because of the wide range of topics and work, it was agreed that each of the five tasks will start with the preparation of a feasibility study to identify the specific sub-tasks necessary to achieve the stated objectives.

4.3.2 Objectives

Objectives of the various tasks in this work package were to prepare new interface specifications for topics not covered in the CAPE-OPEN project. This work package had 5 tasks, 4 to be performed in the EU part of the project and one to be performed in collaboration with the partners from Japan. In Task WP2.1, it was agreed to develop 2 new thermo-properties interfaces. In task WP2.2, a new interface for kinetic phenomena was to be developed. In task WP2.3, under solvers, it was decided to develop interfaces for MILP (mixed integer linear programming), MINLP (mixed integer nonlinear programming) and PEDR (parameter estimation and data reconciliation). Under task WP2.4, it was decided to develop interface specifications for PDAE systems and solvers. Finally, in Task WP2.5, it was agreed to develop “Other Standards” dealing with process engineering activities during the early phase of the conceptual process design.

4.3.3 Technical Progress and Achievements

All the objectives have been achieved. Some of the scopes of the tasks have been revised and some tasks have been combined.

TASK 2.1 PHYSICAL PROPERTIES OF COMPLEX MIXTURES

CAPE-OPEN Thermo Interfaces did not cover handling of complex and ill-defined mixtures. Specifically, the requirements for dealing with petroleum assays, petroleum fractions, electrolyte systems, polymers and particulate materials were not considered in the interface design and definition.

The feasibility study (W211) identified two complex mixtures, petroleum fractions and electrolyte systems for development of new interface specifications and prototypes. Interface specification for complex mixture 1 (petroleum mixture) has been developed together with a limited scope prototype. A revised interface specification draft (W215) for complex mixture 2 (electrolytes) has been developed. After review of the initial interface specification documents for electrolytes and kinetic phenomena, it was agreed in a joint meeting between partners involved with tasks WP2.1 and WP2.2 that the interface specification for electrolytes should be combined with the interface specification for kinetic phenomena. The new combined interface specification for chemical reactions has been developed with limited scope prototypes.

TASK 2.2 KINETIC PHENOMENA

In most process simulators, only thermodynamic state functions and phase and reaction equilibria are treated as separate modules that can be parameterised by the material mixture involved. In many unit operation modules correlations for kinetic phenomena are evaluated in accordance with the material system considered. Most importantly, stoichiometry of chemical reactions as well as chemical kinetics needs to be treated.

A revised interface specification draft (W221) has been developed. However, as reported under task WP2.1, this interface was combined with the interface specifications for electrolytes into the interface specifications for chemical reactions.

TASK 2.3 OPTIMISATION, PARAMETER ESTIMATION AND DATA RECONCILIATION

CAPE-OPEN covered numerical algorithms for the solution of linear and non-linear algebraic equations as well as for differential-algebraic equations. In this task, the objective, identified through a feasibility study, has been to develop additional interface specifications for mixed integer linear programming problems (that also includes linear programming), for mixed integer non-linear programming problems (that also includes non-linear programming) and for estimation of model parameters from experimental data (that also includes reconciliation of plant measurements).

All tasks have been completed successfully. Interface specifications have been developed for MILP, MINLP and PEDR together with corresponding prototypes. The MINLP interface specification draft (W234) proposed major changes in the design of the MILP and MINLP interfaces, which were accepted at the WP2 meeting in London on 10-11 July 2001. The design of these interfaces now follows the same structure of Cape-Open Solver interfaces. The result is a combined interface specification document for MILP and MINLP, which has also been delivered.

TASK 2.4 DISTRIBUTED INFORMATION

The mathematical modelling of systems involving distributed information naturally gives rise to mathematical models described by sets of partial differential and algebraic equations (PDAEs). In WP2.4, we view a system of PDAEs as an object that will be used by a PDAE solver or a discretisation tool. The work done in this WP concentrates on the definition of the interfaces presented by the PDAE system and the PDAE solver.

Based on the document "Scope, concept and interface specifications" document, it was agreed to combine the interface specifications for PDAE Systems and PDAE Solvers into one interface document. The combined W241 + W243 (Interface specification draft for PDAESO) has been delivered. The final interface specifications together with prototype have also been developed.

TASK 2.5 IDENTIFICATION OF FUTURE STANDARDS

WP2.5 is in charge of the Other Standards, which GCO has to look into in order to provide a complete service to the process engineering related activities during the early phase of the conceptual process design. Among them the first attention is given to the area of (1) Process Representation Method and (2) Process Economic Analysis based on a Japanese domestic IMS work. This task is composed of two subsets of work-packages: 1. Process representation method and 2. Process economic analysis. A feasibility study to define the scope of the work has been carried out. Meetings with GCO partners involved with WP6 has also been held to formulate and define the overlap between WP2.5 and WP6.1. Collaboration between the two WPs has led to the definition of stages of the process life cycle through an agreed activity model and to work on a case study where the process representation method and the process economic analysis can be highlighted. Basic Specifications for software interfaces bridging between Process Analysis and Process Design as well as Economic Analysis has been developed based on modeling technique (UML) used by international WP activities. The results and the findings of the study has been documented in a report prepared for the GCO-project (GCO-WP2.5 Final Report).

4.4 WP3: Development of CO-compliant Software

4.4.1 Overview of Work

The CO-compliant software work package had one major responsibility divided in three tasks: developing of CAPE-OPEN compliant software by

- vendors (task 3.1),
- academics (task 3.2) and
- operating companies (task 3.3).

The second responsibility was the development of an interface for a Physical Property Data Bank (PPDB) within task 3.1. Beside the European partners (AspenTech, BASF, DECHEMA, DTU, ELF, Hyprotech, IFP, INPToulouse, Norsk Hydro and RWTH Aachen) also some partners from the US (Honeywell, Air Products and UOP) will develop software either with CO sockets or CO plugs. Under the umbrella of IFP also so-called SMEs (Small and Medium Enterprises) like Belsim, Infochem, Prosim or PSE, contributed with their CO- developments to the success of this work package.

4.4.2 Objectives

Objective of this work package was to stimulate various developments of software modules which are compliant with the Cape Open standards.

Thus the work is mostly dominated by individual software components, that do not interact at all with other developments done in these tasks.

Especially the work done by operating companies in task 3.3 is confidential to a certain extent and will not be disseminated to other partners neither during nor after the project time span. Nevertheless adequate procedures assured that the contracted work in these task had been executed.

4.4.3 Technical Progress and Achievements

As shown in the final meeting in Cambridge almost all partners contributed to the success in this work package. Delays occurring during the time span were overcome as the final date was reached. Also one major concern, the insufficient performance of the Cape Open Interface, diminished as the results of the interoperability team were published. It is common understanding nowadays, that it is not the Cape Open interface, which gives a penalty on the performance. It merely was the kind of applying and coding the interface software. Ways for effectively coding the Cape Open standards are now made publicly available

PPDB Interface

This has been intensively discussed with contributions from many partners worldwide. During the project period we already released version 9 of this software, which indicates the vivid interactions between Dechema and testers.

Vendors

The vendors delivered sockets for unit operation and thermodynamic interfaces, which will enter into their commercial available software versions. The vendors indicated there ongoing interest after official end of Cape Open to continue support existing Cape Open standards and develop further interfaces.

Academics

The academic partners fulfilled their tasks in this work package as scheduled in the workplan.

Operating companies

Like the academics the operating companies mostly achieved their scheduled contribution. see Documents next section. We specifically appreciate the work undertaken by the American partners.

4.5 WP4/ Integration of Open Simulation in the Work Process

4.5.1 Overview of Work

The Integration of Open Simulation in the Work Process work package had three sub-tasks: Work Process and Case Studies (task 4.1); Component Selection and Configuration of Open Simulation Environment (task 4.2); Test and Validation of Open Simulation Environment (task 4.3). As the project proceeded and the simulator vendors announced initial versions of CAPE-OPEN-compliant products, the emphasis of the work shifted from WP4.1 towards WP4.3. This was indicated by the formation of the Interoperability Task Force (ITF). The ITF was charged with facilitating the delivery of practical, plug and play interoperability within commercial flowsheet simulators, via industrially-relevant test scenarios and the critical review of the CAPE-OPEN interface specifications for ambiguities and omissions. This capability within mainstream commercial flowsheet simulators is a prerequisite for acceptance of open simulation in the work place and so ITF activities became the major focus of the work package for the rest of the project.

Representatives from BP, Dow, ICI, IFP and RWTH.IS attended the kick-off meeting for this work package and AspenTech, Hyprotech, Norsk Hydro, JGC and MCC subsequently indicated their intention to participate. After the formation of the ITF, the main contributors to the work package were AspenTech, BASF, BP, Hyprotech, IFP, Infochem, RWTH.IS and TotalFinaElf.

4.5.2 Objectives

Objectives for the work package were:

- To agree a work plan based on the deliverables in the Project Proposal
- To facilitate the provision of practical plug and play interoperability in commercial simulators using CAPE-OPEN interfaces
- To produce an analysis of the impact of open simulation on the work process
- To research the techniques of component selection and produce prototype implementations

4.5.3 Technical progress and Achievements

All of the above objectives were achieved. The work plan was agreed to be incremental, so that it could be easily adapted to changing circumstances in the project as a whole. It was also agreed that this work package was closely associated with work package 8, since the CO-LaN would be the vehicle for supporting open simulation in the work process after the end of Global CAPE-OPEN. The initial work focused on reviewing work practices in participating companies (WP4.1, with Dow, ICI, IFP, Norsk Hydro, JGC and MCC) and on component selection (WP4.2, by RWTH.IS) in the context of the CO-LaN technical vision (WP8).

Once initial commercial versions of CAPE-OPEN-compliant simulators and components became available, it was clear that ambiguities in the CAPE-OPEN Interface Specifications had prevented interoperability from being achieved. For this reason the ITF was formed to provide an independent review forum for the software and CAPE-OPEN interface specifications, in which interoperability problems could be identified and solutions agreed. These solutions were then implemented by the software vendors and the review process repeated by the ITF.

The ITF was approved by the Global CAPE-OPEN Management Committee in March 2001. Its first major objective was to deliver a demonstration, at the mid-term meeting, of the interoperability of steady-state unit and thermodynamic components in AspenTech and Hyprotech commercial software. This was followed by another demonstration at the final meeting, which showed Process Modelling Environments Aspen Plus, HYSYS and gPROMS interoperating with thermodynamic components from AspenTech, Hyprotech and Infochem and unit operation components from AspenTech and Hyprotech. This demonstration was also largely steady-state, but gPROMS also showed a dynamic run. Both demonstrations were given by BP on a BP computer to emphasise the substantial progress that had been made towards routine, intuitive use of open simulation.

The ITF's work plan envisaged the production of a series of Interoperability Scenarios, which detailed the steps that must be followed to allow a process engineer to make practical use of open simulation in different areas of simulation. They were seen to be key documents that provided a bridge between the general software engineering of the CAPE-OPEN Interface Specifications and the particular needs of process engineering end users. The first scenario produced dealt with the use of unit and thermodynamic components in a steady-state, sequential modular simulator. This scenario was tested on a BP computer, using the CAPE-OPEN-compliant simulators from AspenTech and Hyprotech, during two ITF workshops. The list of issues that arose from these workshops led to substantial software improvements, which enabled an interoperability demonstration to be given at the Mid-term Meeting. The process was continued until all the issues with this scenario were resolved and the results demonstrated at the Final Meeting. Problems with clarity and omissions in the Unit Operations and Thermodynamics and Physical Properties Specifications were also addressed in the Version 1.0 drafts that were produced.

As well as the connection with work package 8 already described, the ITF also interacted with the Methods & Tools group and the Project Manager for software engineering and specification change purposes.

The ITF consisted of BP, AspenTech, Hyprotech and TotalFinaElf (as WP 8 leaders) as core members, with BASF, IFP and Infochem joining to provide specific expertise. It addressed the objectives of WP4.3.

In parallel with these interoperability activities, RWTH.IS developed techniques and prototypes to deal with the component selection issues that will arise when the CAPE-OPEN component market becomes more fully established. The description of techniques included the types of component information needed to support efficient component selection, different approaches to the management of component data, data retrieval techniques and a short discussion on implementation approaches. A prototype was produced that demonstrated these techniques, including the use of ontologies to give a more intuitive and flexible search capability.

This work was delivered via 2 physical meetings of the whole work package, i.e. at the Kick-off Meeting and the Mid-term Meeting, 4 ITF workshops, 2 meetings of BP and AspenTech, 3 meetings of BP and PSE and 15 phone conferences. In addition, 6 software interoperability test exercises were carried out at BP.

4.6 WP5: Open Support Tools and Technologies

This work package was one of the main research activities in GCO and its goal was to develop support Tools and Technologies from various perspectives. Universities who currently develop innovative architectures and techniques extended these, taking advantage of the facilities provided by open standard interfaces. Users provided feedback on operational use of the newly developed modules, and vendors took care of ensuring that the modules can be easily integrated with their commercial offers.

The Work-Package was divided into three tasks:

Generalisation of Model Structuring: This sub-task provides a conceptual framework for the structuring of models beyond the unit level. Different types of sub-models are introduced, they are characterised by a list of properties and related to each other by semantic links.

Research on supporting the modelling process.Task: This task addresses model exchange formats, symbolic model transformations, and automated analysis functions, model generation and other supporting tools. Prototypes have been developed in a component framework.

Discrete and Hybrid Discrete-Continuous Unit Operations: The interface definition for units in CAPE-OPEN has been restricted to purely continuous dynamic models. An extension of the standard to hybrid models is carried out in this task. Appropriate interface structures and model prototypes have been developed for Unit Operations, Scheduling and Planning, Operation and Control.

4.6.1 Scientific and technical description of the results

TASK 5.1 & 5.2

The main objective of WP 5.1 and its deliverables D512 and D513 are to enable interoperability of software tools for modelling and model analysis. The effort undertaken comprises the development of a homogeneous data model and an associated exchange language in ASCII format that can be translated into different proprietary formats (e.g. gPROMS, ACM, or Modelica) or that can be used natively by process modelling tools. Tools addressed by these aims are interactive modelling tools such as Model.LA, ModDev, or ModKit. Also, smaller units of functionality (e.g. software components) for model analysis and modifications (degree of freedom analysis, structural index and solvability analysis, or index reduction) could deal with such a format.

As it turns out that the level of granularity in the CAPE-OPEN numeric component design is too high with respect to the performance requirements in the numeric computations domain, a different approach might be to enable interoperability for the problem definition instead of the solver implementation. Feeding a symbolic model to a solution approach has the potential benefits of making a symbolic pre-processing possible, as e.g. required for global optimisation.

A quite different purpose that could be fulfilled by such a format is to increase the description mechanisms of a CAPE-OPEN unit operation component, for example. A unit or ESO component could be asked (e.g. via an additional optionally supported interface) for a description of the model encoded into it and return the model in the format proposed here. This approach is feasible for any CAPE-OPEN components containing a model (also thermodynamics, equation set objects, etc.).

The approach taken from a general modelling language towards a modelling language for process engineering applications is as follows:

1. Define a basic object model offering mathematical concepts like variables, equations, and operators

2. Define an object model for a model of a structured system, model. This level should provide aggregation and decomposition facilities for convenient modelling of technical systems.

3. Define object models for process engineering concepts like units and streams. A material object is associated to them, representing the processed compounds.

4. Define object models for plant objects such as reactors and distillation towers The base of the overall process (items 1 and 2) are a generic modelling language which is rather focused on mathematical concepts which are not specific to process engineering. However, the process-engineering domain motivates the scope of these concepts (i.e. hybrid discrete-continuous systems, distributed parameter systems). The core language is described in the deliverable documents of this two tasks. Further documents (and efforts) concentrate on the other steps explained.

Prototypes have been developed and presented during the final meeting in Cambridge (UK) at the end of 2001.

TASK 5.3

Work package 5.3 is concerned with the modelling of “Discrete and Hybrid Discrete-Continuous Unit Operations”, “Scheduling and Planning” and “Operation and Control” Aspects.

Almost all process systems of practical interest are hybrid in nature, exhibiting both discrete and continuous characteristics. Within relatively narrow ranges of operating and environmental conditions, the fundamental laws of physics expressed in the macroscopic scale (which is normally of interest to process engineering) naturally give rise to continuous mathematical descriptions. However, outside these ranges, discontinuous behaviour arises routinely due to phase transitions, flow regime transitions, equipment geometry and a vast variety of other factors.

Discrete/continuous behaviour is an intrinsic characteristic of most process systems even when subject to continuous external inputs. The latter comprise a variety of disturbances, over which we have no control, and deliberate control actions and manipulations imposed on the plant as a result of process operation and control. Of course, in reality, these inputs may themselves be discontinuous and in general may depend on the state of the process itself. Indeed, any process that is operated in an essentially dynamic manner, such as a batch process or a periodic separation process, will experience frequent control actions of a discrete nature in order to maintain operation in a time dependent, often cyclic, mode.

In general the description of hybrid discrete/continuous process systems can be decomposed into two distinct areas: modelling the fundamental physical behaviour and modelling the external actions imposed on this physical system. Work Package 5.3 A, B, C is concerned with the latter and aims to define standard interfaces for operating procedures for modelling external manipulations of process plants consisting of one or more unit operations.

The schedule given above has been almost followed. Discrete/Hybrid Interface Specifications Draft for "Scheduling and Planning" have been submitted to an RFC at the beginning of 2001 as well as the part concerning the "Operation and Control". Draft interface documents of part B and C have been uploaded on the BSCW and submitted to an RFC. Prototypes of part B and C have been made available mid August as well as Final Interface Specification document. Concerning the “Discrete and Hybrid Discrete-Continuous Unit Operations the Draft Interface document is available in the BSCW and the prototype has also been recently made available. A Demonstration of Parts A and B was carried out at Cambridge Final Meeting.

The prototypes document gives an overall structure overview. Then the original problem is described and the way in which the information is sent from the client to the server is described, the wrapping work carried out is briefly explained. Conclusions and comments are presented, in order to provide feedback to the interface specifications. Besides, the appendix includes the instructions for running the prototype. The prototype, the source code and the corresponding documentation in html format are also available at the BSCW.

The work presented in this contribution interprets the objective of work package 5, supporting the modelling process, by providing interoperability between modelling tools. Though this can also be achieved by specification of component interfaces, the specification of a suitable file format seems to be more promising and is closer to the current implementation of modelling support tools. To make a proper problem analysis, a neutral object model is proposed first. Using modern technical standards, the object model proposed is represented using XML to yield a neutral model exchange language. Possible uses are identified and a critical assessment is being made.

Discrete and Hybrid Discrete-Continuous Unit Operations

Documents describing Hybrid Unit Operations Interface Specifications Draft (W531A) and corresponding prototype (D532A-UO) as COM client have been delivered (UPC). Also, a Demonstration of Parts A and B was carried out at Cambridge Final Meeting.

Scheduling and Planning

This document describes the Interface Specifications for the Scheduling and Planning Package of the Global CAPE-OPEN Interface System. The document starts with a text description of the requirements identified for a scheduling and planning component. Then is expressed in Unified modelling Language and developed into a specification of the interfaces necessary for a CAPE-OPEN (CO) planning and scheduling component to be used by a CO executive by means of its interfaces. These specifications are provided in both COM and CORBA IDL.

The GCO main objective is to provide an Interface System as standard for the communication between different software components that carry up different tasks. For example, Planning & Scheduling Component to any compliant CO Executive, which performs the co-ordination and the connectivity between the different components available in one system. The goal of the Interface is to translate the requests for information or action, given by one of the components involved, into something any other component understand. In addition, the interfaces developed should be flexible enough to incorporate the latest developments in the scheduling area and to make possible the access to the component specific information. The minimum information that should be accessible to all components will be defined according to the standards ISA S95 and ISA S88.

The Interface can be thought of as a "socket" and a "plug", which are capable of exchanging information between them. The Executive and Planning & Scheduling Component do not need to know anything about the internal architecture of the other. This last point is very important in the planning and scheduling area since there is no standard method used in the industry but rather a lot of site-specific solutions exist. In this respect the Scheduling and Planning standard *interface* has to be as open as possible, defining the minimum information flow and functionality required to be accessed from other components and providing also a way of communicating with the information and calculation capabilities of each specific implementation. Reference is also made to the use cases developed by the CAPE-OPEN Numeric Work-Package.

4.6.2 Results and conclusions

As we mentioned in the introduction, this Work-Package is one of the main research activities in GCO. Work Items Documents and Deliverable Documents planed have been finished and published within the project, except for Part A of task 3. Work done in this Work-Package has been demonstrated during final GCO meeting in Cambridge. All demonstrations made during this meeting are based on prototypes. What can be envisionable now is to integrate this work into commercial offers (into CO-PME) for “Operation and Control” and “ Scheduling and Planning”. The CapeML object model will mature and could evolve to a standard of model exchange/transformation/Unit Generation.

4.7 WP6: Advancing Open Process engineering

4.7.1 Overview of Work

Tools for Computer Aided Process Engineering (CAPE) no longer run on isolated machines. They rather provide information, which can, and should be shared over a network: an Intranet or the Internet. Work package 6 looked at how CAPE tools can participate in an open way as information providers and users in a distributed engineering environment. The work was partly an analysis and evaluation of input and output data in typical process engineering tasks, and partly software prototype demonstrations.

The work package was research-oriented and was divided into four parts:

- Subtask 6.1.1: Develop a data (flow) model to support and enable the use of process models through the process lifecycle.
- Subtask 6.1.2: Develop a data (reference) model to support and enable the use of process models in distributed simulation environments.
- Subtask 6.2.1/2: Develop the conceptual basis of integrating simulators and optimisers in a real-time environment for the support of process operations.
- Subtask 6.2.3: Develop a data (flow) model to support open process simulation with polymers

4.7.2 Objectives for the work

The main objectives for the work were:

- Identify, design and demonstrate lifecycle modelling interface requirements (Subtask 6.1.1)
- Plan and design prototype demonstrations of open process simulation (Subtask 6.1.2)
- Identify data flows and develop and test out a reference model for real-time simulation (Subtasks 6.2.1 and 6.2.2)
- Identify requirements and data flows for polymer simulation. (Subtask 6.2.3)

4.7.3 Technical progress and Achievements

Generally, documents and prototypes have been delivered as planned. However the scope of this research-heavy work package has been somewhat changed during the project. This must be expected because a) the work package involve research and development and b) the work package duration has been three years and several key persons have been replaced. Most documents have been delivered as planned, but two deliverables have been merged and one deliverable has been replaced by a different document. Several additional documents and prototypes have been delivered. Two of these concern the new subtask 623, but additional deliverables for all parts of the work package have been made.

For subtask 6.1.1 two realistic and industrial-size case studies have been presented and data flows in the lifecycle have been identified (D611). Lifecycle interface requirements have been derived and presented (D612). Some interfaces for the exchange of data between different application tools used throughout the design lifecycle of chemical processes have been described (D613). The results have been illustrated through two software prototype demonstrations, one using Methyl Acetate production as case and another using Nylon6 production as case.

For subtask 6.1.2 open, hybrid, distributed process engineering have been demonstrated. A CORBA CAPE Open Unit skeleton (D617) has been developed and used to produce two CORBA CAPE OPEN unit models (defined as deliverables of work package 3). These units are included in a prototype demonstration (D619) of hybrid process simulation between Unix and Windows using a simple modelling environment (D618). Once a robust, commercial COM-CORBA bridge becomes available the unit modules may be run using commercial version of Process Modelling Environments such as

AspenPlus or Hysys. One of the CORBA CAPE OPEN units is a wrapping of a Fluent Computational Fluid Dynamics (CFD) simulation, and was done in co-operation with resources from task 2.4. This prototype with communication between Computational Fluid Dynamics (CFD) model running on Unix/CORBA and a Cape Open simulation executive running on Windows NT/COM indeed advances open process simulation.

For subtask 6.2.1 data flows in a real time environment (D621) have been analysed. A reference model document has been delivered (D622). The results have been illustrated and verified through a software prototype demonstration of pilot plant operation. The prototype includes a real-time event handler and controller as well as scheduling and planning. The requirements for and the specification of interfaces to be used for interaction with and simulation of real time environments have been described (D623/4). The interfaces provide methods for reading from and writing to external data sources. and methods to control a simulation from an external program.

A demo was realised in Cambridge Meeting integrating simulators and optimisers for supporting process operations in real-time that uses CORBA CO-compliant interfaces for Planning and Scheduling (WP 5.3B), co-ordination system (WP 5.3C), Hybrid simulation (WP5.3A), Data reconciliation (WP2.3) and MILP solver (WP2.3). A JDBC interface was used to access a common database.

Additionally, requirements for open polymer process modelling, simulation and operation have been identified within task 6.2.3 jointly by UPC and ICI. This includes a requirements document (D625) where future interfaces for polymer physical property packages, polymer kinetic models and batch polymer process optimisation are presented. A report (D626) describes the modelling of a polymer case study that identifies the different requirements present in practice.

4.8 WP7: Dissemination

OVERVIEW OF WORK

The Dissemination work package has four major responsibilities: defining the CO opportunity to software providers (task 7.1); defining the CO opportunity to software users (task 7.2); establish and maintain relationships with relevant organizations (task 7.3), and communicating the CO opportunity to software users and providers. In this section, we briefly outline some achievements of the work package in terms of the Work Package responsibilities.

OBJECTIVES FOR THE PERIOD

Our objectives for the project were:

- To work with WP8 in the development and maintenance of the CO-LaN web page;
- To maintain an active presence for GCO in technical presentations and press releases;
- To maintain relationships with identified key relevant organizations;
- To facilitate GCO members' presentation and publication to the CAPE community.

TECHNICAL PROGRESS AND ACHIEVEMENTS

All objectives listed above have been reached. Dissemination efforts have been very effective through the final quarter of 2000 and all of 2001. Several major conferences have been targets for communicating to the CAPE community, and many presentations and publications have taken place (see list below). GCO summary documents, an FAQ list, and a CO Glossary have been posted on the CO-LaN web site. In addition, a current events page has been maintained on the CO-LaN web site, communicating the dissemination activities to a broad community of CAPE practitioners. Presentations and publications have been shared with GCO project members via the BSCW server. All project documents are stored on the BSCW server. A working relationship has maintained with the American Institute of Chemical Engineers (AIChE) Design Institute for Physical Properties

(DIPPR). Continuous communications are maintained with the other GCO Work Package Leaders regarding current and future Dissemination opportunities. The Exploitation Committee was established, a work plan developed, and activities under this committee completed. Finally, with GCO Support funding, the first edition of the CAPE-OPEN Update newsletter was published in early 4Q01.

During the first 15 months of the GCO project, Dissemination activities were not funded by the EC, so all of the work of this WP was the result of "in-kind" effort on the part of those preparing, reviewing, submitting, publishing, and presenting the information. With the initiation of the GCO Support project in June, 2001, funding was available for support of the CAPE-OPEN Update newsletter, the web site, CO Tour days, and other related activities. In October 2001, the first edition of CO Update was distributed to over 1000 CAPE practitioners via e-mail. Since September 2000, additional presentations have been made at a number of conferences and meetings, including the following:

- CAPE-OPEN day, Cambridge, UK, December 2001
- Multiple papers presented at AIChE fall meeting, Reno, Nevada, USA, November 2001
- Presentations at SIMS 2001, Porsgrunn, Norway, October 2001
- Presentation at SIIT2001, Boulder Colorado, October 2001
- Presentation at 6th World Congress of Chemical Eng., Australia, September 2001
- CAPE-OPEN day, Milano, Italy, September 2001
- Presentation at ECCE3, Nuremberg, June 2001
- Presentation at DYCOPS 6, Korea, June 2001
- Presentation at ICheaP-5, Florence, Italy, May 2001
- Presentations and demonstrations at ESCAPE 11, Kolding, Denmark, May 2001
- Presentations and demonstrations at PPEPPD, Kurashiki Japan, May 2001
- Presentation at Bridging the Gap, Sweden, May 2001
- Article in US AIChE CAST Newsletter, US, April 2001
- Presentation at CAPE-21 workshop, Delft, February 2001
- Presentation at Norway Oil & Gas meeting, Oslo, February 2001
- Books on Computer Aided Chemical Engineering Series, published 3Q 2000
- Presentation at ENSIGC & EMAC courses, France, December 2000
- Presentations at SUSTECH 11 CAPRI, November 2000
- Presentation at IMPROVE, Aachen, Germany, November 2000
- Multiple papers presented US AIChE fall meeting, Los Angeles, November 2000
- Presentation at DIPPR , Los Angeles, November 2000
- Presentations and demonstrations at Hyprotech2000, Amsterdam, November 2000
- Presentation at 50th Canadian Congress Of Chemical Engineering, Montreal, October 2000
- Presentation at ECCE'2, Montpellier, France , October 2000
- Article in Ernst & Young E-Journal, www.businessinnovation.ey.com, September 2000
- Article in Chemical Engineering Progress, September 2000
- Presentation at ATOFINA science and engineering conference, September 2000

Press releases have been issued as follows:

- GCO final project summary, January 2002
- Invensys/SIMSCI support for CO standards, January 2002
- CAPE-OPEN 2001 Award (Dr. Siegfried Nagel), December 2001
- Process Systems Enterprise (PSE), Virtual Materials Group (VMG), BelSim, and the AIChE's Design Institute for Physical PRoperties (DIPPR) join the CO-LaN, August 2001
- Establishment of CO-LaN, February 2001

These activities have served to significantly raise awareness of the CO concept and principles and the activities of the GCO project. The next opportunity (for the EU funded GCO Support project) is to stimulate a vibrant market place for CO compliant software in the CAPE community. It is clear from comments and questions that GCO partners receive from the CAPE community that we have accomplished the goals of this Work Package.

4.9 WP8: CO-LaN

4.9.1 Overview of Work

The CAPE-OPEN Laboratories Network work package had three subtasks: Master Plan and Lab Development (WP8.1); Migration Tools and Cookbook (WP8.2); Test Procedures (WP8.3). As the project proceeded, the involvement of some partners in work package 8 shifted to other activities or was reduced. Especially vendors preferred to realize their development activity around Migration Tools within WP1 rather than within WP8.

4.9.2 Objectives

Objectives for the work package were:

- To create a CAPE-OPEN Laboratories Network
- To provide tools in order to facilitate the use of the CAPE-OPEN standard
- To provide tools to test the compliance of applications with the CAPE-OPEN standard

4.9.3 Technical progress achievements

All the above objectives were somehow attained if not in due time.

The CAPE-OPEN Laboratories Network (CO-LaN) was incorporated in February 2001 after elaborating a Master Plan among the partnership. The objective of three labs, one in each main regions was dropped for the moment. During 2001, a number of software vendors joined the CO-LaN but the main software vendors, AspenTech and Hyprotech were reluctant to join. A competing initiative called CAPE-S was even launched by AspenTech before being dropped but this led to a modification of the CO-LaN motives, missions, objectives and membership by the end of 2001. These modifications were formally agreed on March 22, 2002 in Frankfurt, Germany. Still the CO-LaN is active, disseminating about the CO standard, advancing the standard, developing testing facilities, and mostly defining user priorities in regard of the CO standard.

The CO-LaN has its own web site facilitating dissemination and shared work: www.colan.org. It is presently hosted by RW2 which serves as web administrator.

Migration tools have been mostly developed within WP1 by AspenTech and Hyprotech while RW2 has developed a generic migration tool for FORTRAN legacy code. AspenTech and Hyprotech migration tools, respectively a UNIT wizard and a THERMO wizard are made freely available by their developers, either through their web site or the CO-LaN web site. The migration tool from RW2 will be made shortly available from the CO-LaN web site.

A migration cookbook has been released at the end of March 2002 by RW2 and is downloadable from the CO-LaN web site. It helps developers understand where to focus their work.

The self-learning tool is just a prototype which is not made publicly available. The e-learning aspects of this deliverable have not been mastered in time with the resources available for it.

The CO Tester suite has begun operation in September 2000 and has been advancing ever since. It can be downloaded from the CO-LaN web site. The CO-LaN has funded the development of a number of testers: testers for COSE sockets of UNIT and THRM, a tester for PPDB plugs, for SMST plugs and more recently work is under way for a tester of MINLP plugs. However, the aim of the CO Tester suite had to be shifted from labelling to compliance testing since first vendors were reluctant to be constrained by an additional label and secondly interoperability testing proved to be very important to reach a complete plug and play operation. The CO tester suite remains as an help to developers and a necessary screening tool before any interoperability testing.

The work was delivered through a number of physical meetings and phone conferences. Physical meetings took place at IFP in Paris and Solaize, in Aachen with RW2, in Toulouse with ProSim SA, one of the companies subcontracted by the CO-LaN to develop testers, in Barcelona with UPC also subcontracted by the CO-LaN to develop testers.

5. Management and co-ordination aspects

5.1 Dedication to the project, motivation, supply of deliverables

IN EUROPE

All partners, even ICI, were contributing to the project with dedication and motivation and supplying deliverables in accordance with the initial or revised plans. The level of co-operation among European partners and between European and international partners was extremely satisfactory. Users, researchers and vendors of CAPE software collaborated fully in order to develop the CO standard.

IN JAPAN

The Japanese consortium was supported by IMS funding. The Japanese activity was concentrated in a number of specific tasks, and their contribution has been very good. The Japanese members participated in the project meetings, committees, phone conferences and other activities, and organised regional GCO meetings for the Japanese partners of the project. Mitsubishi Chemicals properly ensured the co-ordination of Japanese participation.

IN NORTH AMERICA

The US and Canadian consortium were not supported by any funding, and therefore were depending on in-kind contributions from all partners. This made participation harder for universities, who need at least travel funds for attending meetings. For this reason, the US co-ordinator, Dow Chemical, tried to raise funding for supporting the US universities, unfortunately without success. The good side of the project is that several north-American partners were active, attended a training session, participated in phone conferences and meetings, commented documents, and more generally speaking did their best to contribute to the project with the limited resources available. Life would be easier with more funding, of course, but this is a problem that IMS has to face in general, not only the GCO project.

5.2 International co-operation (IMS)

The GCO project operated in the context of IMS. It was therefore important that co-operation take place at several levels between the regions. At Steering Committee level, all partners (except reviewers) participated. At Management Committee level, the three regional co-ordinators and workpackage leaders from EU, USA and Japan were involved. Partners participated in other committees depending on their status (e.g. software vendors in the Exploitation Committee etc.). The work packages and tasks groups involved contributors from all regions, depending on their interest and resources, rather than depending on their geographical situation. The electronic BSCW collaboration server was accessed by all partners world-wide. All partners world-wide were trained to CO technologies in the first year of the project.

In summary international co-operation took place in GCO at every level.

5.2.1 Communication and logistics

The project used conventional and advanced communication facilities as CAPE-OPEN did, including the main collaborative workgroup server. There was no exchange of paper or faxes in GCO, except for contractual matters.

BSCW AND WEB SERVER, EMAIL

The GCO BSCW collaborative workspace, http://Sunsite.informatik.rwth-aachen.de/bscw/bscw.cgi had up to 80 registered users. It was a key element of the project, as it allowed the sharing of all project documents through the web. Now it constitutes the project's memory.

The GCO web site, www.global-cape-open.org , was a minimal web site aimed at making the CAPE-OPEN interface specifications publicly available and giving brief news. It was replaced in 2001 by the www.colan.org web site, the website of CO-LaN, which is developed thanks to GCO-Support accompanying measure funding.

TELECONFERENCES

During GCO, teleconferences were organised for:

- The management committee (one per month, around 30 in total);
- The scientific and technical committee (depending on needs);
- The Methods and Tools group (one per month, sometimes less, 20 in total);
- Specific work packages (see their individual reports).

Such teleconferences gathered from four to twelve participants for one or two hours. They were minuted and minutes were distributed to the partners.

WORK PROCESS

The work process that was defined in CAPE-OPEN was used in most tasks by GCO. The GCO work process included an approval process that was defined in the first months of the project and delivered in November 1999.

5.3 Meetings

5.3.1 Steering Committee Meetings

The Steering Committee was composed of high-level representatives and met once a year. They first met on Nov. 10th, 1999 in Brussels. This meeting was mainly used to give GCO activity a higher priority level within the participating organisations. They met again on Nov. 8th, 2000 in Amsterdam, and on Dec. 5th , 2001 in Cambridge, UK. The list of European and international Steering Committee members is:

- Edouard Freund, IFP, Executive Vice-President, R&D; chair of Steering Committee
- Bruno Wiltz, Atofina, Executive Vice-President for Technology, Engineering and Energy
- Prof. Xavier Joulia, INPT
- Frank Whitsura, UOP, General Manager of Engineering
- Erik Gran, Norsk Hydro, Section head, Corporate Research Centre
- Prof. Jorgensen, DTU, Co-director of CAPEC
- Prof. Sigurd Skogestad, head of department and leader of NTNU's CAPE Center
- Prof. Luis Puigjaner, UPC, professor and chairman of Chemical Engineering Department
- Andrew Ogden-Swift, Honeywell Hi-Spec Solutions, Director of Technology Management
- Dr. Thomas Bott, BASF, Abt.Direktor
- Gordon Hutchinson, BP, Head of Engineering
- Prof. Wolfgang Marquardt, Director of RWTH.LPT
- Prof. Matthias Jarke, Director of RWTH.IS

- Salvador Clavé, AEA Engineering Technology Hyprotech, V.P. European and Middle East Operations Manager
- Rainer Gawlick, AspenTech, VP Product Marketing
- Prof. Costas Pantelides, Deputy Director, Centre for Process Systems Engineering, Imperial College
- Werner Merk, Dow Chemical, leader of process modelling.
- Takeshi Ishikawa, Mitsubishi Chemical, General Manager of Science & Technology Office.

5.3.2 Management Committee Meetings

The Management Committee had physical meetings every four months in addition to the monthly conference calls. One meeting was held in Brussels and was partly attended by the EC scientific officer.

The members of this committee were the project co-ordinator, the regional co-ordinators from USA and Japan, and the work package leaders.

5.3.3 Scientific and Technical Committee Meetings

The Scientific and Technical Committee had three physical meetings in addition to the phone conferences. It disappeared after the midterm meeting, since all Sci & Tech questions were dealt with. The members of this committee were the representative of all academic and software suppliers partners, plus the representative of TotalFinaElf as co-ordinator (after an initial period chaired by the representative of Norsk Hydro).

5.3.4 Exploitation Committee

The Exploitation Committee was created around May 2000 and dealt mostly with Exploitation matters. Its task was to raise CAPE-OPEN matters in the priorities list of software vendors.

6. Results and Conclusions

The press release written after the final meeting is the best conclusion we can think of:

Global CAPE-OPEN raises the CAPE-OPEN standard to a new level

The Global CAPE-OPEN project had its final meeting in Cambridge on 5th/6th December in an event hosted by AspenTech UK Ltd. This marked the end of five years of international EU-supported work on the establishment of open standards for flowsheet simulation, at first in the CAPE-OPEN project and then in the joint EU/IMS Global CAPE-OPEN project. The results, shown in the meeting, exceeded all expectations.

The aim of the projects was to define standard plugs and sockets so that external software components can be used in Lego™ brick plug and play fashion in the main commercial simulators, such as AspenTech's Aspen Plus and Hyprotech's HYSYS. Although the original project scope did not commit to the delivery of commercial implementations of the standards, this is in fact what has happened in the areas of unit operations and thermodynamics. Developers at AspenTech and Hyprotech, who have been central to the implementation and refinement of the standards, have incorporated them into the latest versions of their simulators. Specialist suppliers PSE and Infochem have also produced compatible versions of their respective gPROMS process modelling environment and Multiflash thermodynamics packages, which will be issued shortly. All of these were demonstrated working together reliably and intuitively, by an industrial end user. Other suppliers, such as ProSim, Belsim, RSI, and Dechema, are expected to provide the same level of interoperability in their products shortly. Open simulation is now a commercial reality.

As well as these commercial implementations, many other facilities were shown in an advanced state of development. For example, there are wizards to enable existing code to be wrapped into CAPE-OPEN-compliant components for both unit operations and thermodynamics and testers to check components for CAPE-OPEN compliance. There are also specifications for numerical methods, petroleum materials, electrolytes, reactions, on-line and hybrid applications, as well as research work aimed at real-time operations, scheduling and planning, and plant lifecycle issues.

Besides these technical developments, the projects have changed the relationships between the participants. All have found that strong collaboration and mutual understanding are essential to deliver the standards and prototypes, while continuing to compete vigorously in all other areas. There was wholehearted agreement with Dr Bertrand Braunschweig from IFP, the project manager of both projects, when he said, "The challenge for the future is to realise the commercial benefits of the hard work and investment of the last five years, but now is the time to celebrate!"

Full details of the standards, the current state of implementation and the project organisation can be found at www.colan.org, which is the web site of the CAPE-OPEN Laboratories Network. This is a not for profit organisation, which has been formed to maintain and develop the standards into the future.

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