1. Introduction

CAPE (computer-aided process engineering) tools are essential for getting products and processes quickly to the market, but the incompatible and proprietary nature of commercial simulators has resulted in a number of significant deficiencies:

- hard to include company specific models and process knowledge,
- need for multiple simulators, with additional license fees, training, and error prone data transfer,
- hard to incorporate the expertise of researchers and specialist companies in simulations
- difficulty in integrating niche software products from small and mid-size enterprises.

The objective of the Global CAPE-OPEN project is to deliver the power of component software in CAPE. CAPE-OPEN promoted the advent of open-standard interfaces for process simulation, which allow users of compliant simulators to employ elements from other suppliers directly in their simulations, without any programming or the production of special versions, and allow covering the full process life-cycle with compatible simulation. We present the CAPE-OPEN interfaces and show how these interfaces enable seamless interoperability of unit operation models and thermodynamic packages in CAPE-OPEN compliant Simulator Executives (COSEs). We then introduce the CAPE-OPEN Laboratories Network (CO-LaN), a non-profit organisation in charge of maintaining the standards and of giving compliance labels to process modeling components.

CAPE-OPEN and Global CAPE-OPEN are funded by the European Community under the Industrial and Materials Technologies Programme (Brite-EuRam III), under contracts BRPR-CT96-0293 and BPR-CT98-9005. In addition, Global CAPE-OPEN follows the Intelligent Manufacturing Systems initiative promoting collaboration between six international regions
2. **End User Needs**

In today’s tough, competitive world, survival demands excellence in process design and operation. Excellence requires more precise knowledge and evaluation. Precision requires effective simulation tools. Benefits are typically quoted as 10c to 25c. per barrel of feed. Ultimately, survival is priceless.

Scope of simulation has been widely spread. Using only one simulator for all activities throughout the process life cycle is no more possible. Process companies need now to
- Include specific models and process knowledge of specialist in commercial simulators,
- Integrate niche software products from small and mid-size enterprises,
- Use multiple simulators within a company – even within the same department,
- Transfer data from a software tool to another in seamless and error prone manner.

These features are clearly not easily provided today by simulation vendors. Moreover, companies are spending a lot of money in selecting amongst general-purpose simulation tools, in their installation, training and maintenance. How awful it is for a decider to make the appropriate choice for his life! You know how long it takes to change from one simulation provider to another.

Simulators need definitely to evolve towards opening and interoperability. Open-standard interfaces are required, which allow users of compliant simulators to employ in-house models and elements from other suppliers directly in their simulations, without any programming or the production of special versions.

Customer demands and modern software technology are driving toward a common software system that can be used for the different simulation purposes throughout the life cycle of the plant.

3. **The CAPE-OPEN standard and the Global CAPE-OPEN project**

CAPE-OPEN was a collaborative project sponsored by the European Commission under the Industrial and Materials Technologies Program from January 1997 to June 1999. The objective of the project was to develop open interface specifications enabling interoperability of process simulation components, and to demonstrate their viability through working prototypes. The partners comprised chemical or petroleum operating companies (BASF, Bayer, BP, DuPont, Elf, ICI), a process licensor (IFP, co-ordinator), major international
vendors of process systems tools (AspenTech, Hyprotech and SIMSCI), European academic research groups in the process systems field (Imperial College, RWTH-Aachen, INP-Toulouse) and a software consultancy (Quantisci). These partners worked collaboratively to develop the specifications and build prototypes.

The project developed standard interface specifications for unit operations modules, physical and thermodynamic properties systems, numerical solvers, graph analysis tools. These specifications have been widely published and are available from the Global CAPE-OPEN Website [2].

The feasibility and industrial potential of the CAPE-OPEN standard is illustrated by two demonstrations: the COM\(^1\) demo developed by the simulation software vendors Aspentech and AEAT-Hyprotech to show short-term exploitation potential; the CORBA\(^2\) demo by RWTH Aachen, IFP, Imperial College and INP Toulouse, to illustrate a path into the future of heterogeneous equation-oriented simulation environments.

The next stage of developing an open architecture for process engineering is the Global CAPE-OPEN (GCO) project, operating as an IMS activity involving interregional collaboration. The partnership in GCO gathers an unprecedented setting of highly skilled users, developers and researchers in CAPE. The partners represent 50% of the world users of CAPE software, 90% of the suppliers, and 10 amongst the top 12 research laboratories on the subject world-wide. The mix of users gives a broad scope including speciality and bulk chemicals, continuous and batch processes, and petrochemical and refining processes. The project develops and uses standards which need a world-wide acceptance, and therefore, contributions from four major industrial regions (EU, USA, Canada, Japan) are needed.

Global CAPE-OPEN has the following key objectives:

- To develop additional standard interface specifications for other components of process simulation: kinetics, complex materials, databases of physical properties, optimisation, data reconciliation, distributed systems, costing;

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\(^1\) Component Object Model, Microsoft's middleware

\(^2\) Common Object Request Broker Architecture, OMG's middleware
To consolidate the CAPE-OPEN results by setting up a management environment for the standard itself, and for the labelling of compliant components, the CAPE-OPEN Laboratories Network, or "CO-LaN";

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).

The first achievements of the GCO project were demonstrated during the project mid-term meeting hosted by AEAT Hyprotech and collocated with the Hyprotech2000 conference in Amsterdam. Painless interoperability of two commercial environments from Aspentech and AEAT Hyprotech was demonstrated, completed by demonstrations of CAPE-OPEN compliant software components from several companies and universities. New standards for additional components were presented, and the foundation of the CO-LaN was proposed.

The second half of the GCO project will further develop these technologies, giving a sound operation basis for the forthcoming CO-LaN initiative.

4. CAPE-OPEN standard interfaces for Unit Operations and Physical Properties components

Unit Operation, Thermodynamics and Physical Properties are among the most frequent calculations carried out in process simulators and it is crucial to consider them in the context of CAPE-OPEN.

Unit Operation software components are the individual building blocks used to create models of the sequences and networks of individual chemical and physical operations that make up a manufacturing process. The accuracy of a simulation is often extremely dependent on the thermodynamics models. Once developed, models are necessary for simulation in the whole
life cycle of a process. Standardised interfaces will enable integration of those models into all appropriate software.

**Unit Operation Interfaces**

The actions of the user during development of a simulation are an important determining influence on the interface between the Unit Operation and the simulator executive. In general, these will include choosing flowsheet blocks, making connections, initializing selected Unit Operations, and specifying feeds and products.

In order to connect Unit Operations in simulation flowsheets, the CAPE-OPEN concept of a port is used. A port is defined as an interface that connects material, energy, and information objects from block to block. Ports are provided by Unit Operations as sockets to which the simulator executive can connect its objects. Ports are the mechanism for information exchange between the Unit Operation and the Simulator Executive, but do not in themselves define the data items to be transferred. This is the role of global and public variables. Global variables are standard names associated particularly with material ports, for example those for temperature, pressure, flowrate and composition. Public variables are defined by a Unit Operation or other flowsheet block and (during solution) can be exchanged via information ports. These variables may also be accessed directly by the simulator executive during configuration and reporting. These names will not be defined by the standards, but means of communicating them will be defined. Global and public variables may either be read/write, or read only; variables which may be set can be used to initialize a Unit Operation or may be reset during solution, for example by an optimizer. Read-only variables may be used in calculation blocks or during reporting.

In fact, the interfaces were designed to follow a tree structure that allows navigating from the top-most interface (ICapeUnit) to the bottom-most interface (ICapeParameterSpec). Every interface is provided with a method that allows the client to access an interface just at the lower following level. Thus, GetPorts and GetParameters return an IDispatch pointer that can be used to query the corresponding ICapeUnitCollection interface or alternatively to query the corresponding ICapeIdentification interface, that provides information about the identity of the entity that represents the collection (i.e. its name and its description).
This tree structure for navigating from one interface to the others is part of the CAPE OPEN standard (and it is reflected in the diagram below). The diagram below shows an overview of the various components in the CAPE-OPEN Interface System and shows the associations between the components, e.g. the UnitOperation component makes use of the PortCollection component, which makes use of the Port component.

Note that the port and parameters collections are represented as two separate components, whereas, in fact, they both use a generic collection component. Also, the diagram is presented in terms of COM. In particular, components are shown using the IDispatch interface of the components with which they interact. IDispatch along with IUnknown provides access to all the interfaces on a component, so the diagram can be shown in a less cluttered form.

Figure 1: Main interfaces
**ICapeUnit**
This interface handles most of the interaction with the unit.

**ICapeUnitEdit**
This interface allows the COSE to display any graphical user interfaces the Unit Operation may have. This interface is not mandatory.

**ICapeUnitPort**
This interface provides access to a units port. These in turn provide access to materials, energy and information streams provided by the host simulator.

**ICapeUnitCollection**
This interface provides a means of collecting together lists of CAPE-OPEN entities such as parameters and ports.

**ICapeUnitReport**
This interface provides access to the reporting facilities of the unit. This interface is not mandatory.

**ICapeIdentification**
This interface provides a means of obtaining the name and description of a CAPE-OPEN component.

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**Table 1: Unit Operation Interfaces**

**Thermodynamic Components**
CAPE-OPEN defined four thermodynamic components. The *Thermo System* is a kind of Property Package manager, that allows end user to define a specific Thermo Property Package. The *Property Package* that can be standalone or generated from the Thermo System. Property Package Creation & Management is the process by which existing Property Packages are made CAPE-OPEN compliant and properly registered. Flowsheet Definition requires that materials be properly defined using CAPE-OPEN Property Packages. These Materials are then assigned to units in the Flowsheet Definition stage. *Calculation Routines* and *Equilibrium Servers* (Flash Calculations) are typically only a small portion of the full property package. The majority of the property package is comprised of the native routines, data, parameters and flash calculations of existing and native Property Packages. The combination of Equilibrium Servers and Calculation Routines, along with the proprietary structure of the property package provide the structure for a CAPE-OPEN compliant property package.
ICapeThermoSystem
This interface allows to generate a specific Thermo Property Package

ICapeThermoPropertyPackage
This interface allows the COSE to display any graphical user interfaces the Unit Operation may have.

ICapeThermoEquilibriumServer
This interface provides access to a specific flash calculation.

ICapeThermoCalculationRoutine
This interface provides a specific property calculation.

ICapeIdentification
This interface provides a means of obtaining the name and description of a CAPE-OPEN component.

Table 2: Thermo Interfaces

Overview
The components defined by this specification are:

Unit Operation: the Unit Operation itself.
Port: is the means by which a unit is connected to its streams. Streams are implemented by means of material objects.
Port Collection: is the means by which the unit groups together its ports.
Parameter: a public parameter is the means by which a component can make its internal variables visible to another component.
Parameter Collection: the collection of parameters that a unit wishes to expose to the outside world.
Thermo System: is the thermodynamic package. It may be built into the simulator or is a CAPE-OPEN plug-in component itself.
Thermo Property Package: is the thermodynamic package. It may be built into the simulator or is a CAPE-OPEN plug-in component itself.
Thermo Equilibrium Server: performs flash calculations.
Thermo Calculation Routine: is used to implement custom thermodynamic calculations
Material Objects: are provided by the simulator and represents flowsheet streams. It also provides access to all thermodynamic calculations.

Table 3: Main interfaces
To be CAPE-OPEN compliant implies for a component not also to implement CAPE-OPEN interfaces but also to interfere with other object and react in a proper way. What follows, as a
corollary, is that every registered CAPE-OPEN standard component, used to deliver the CAPE-OPEN interfaces has to support the ICapelIdentification interface. This is a necessary condition but not a sufficient one, since other non-standardised components used to deliver the CAPE-OPEN interfaces may also implement this interface. This is the case for a component such as Ports. A CAPE-OPEN component has other characteristics, such as that they are registered using CAPE-OPEN mechanisms that make them CAPE-OPEN plug-and-play components.

5. **Implementation**

We are developing software with CAPE-OPEN interfaces. Our applications share business components, and obviously we want to use a middleware solution. We would rather use CAPE-OPEN interfaces than create our specific interfaces. CAPE-OPEN meets our need in Unit Operation and Thermodynamic domains. But the gain is not only to reuse component in other developments, it’s also to decrease some risk in the software development project. Each software developer can now deliver a tested component before integration. Design costs are increased while integration, validation and maintenance costs are decreased. The CAPE-OPEN interfaces are documented (as well as their implementation) in a standard way, this is not always the case when we are using our own component interfaces.

**Technology choice**

We are working under Windows NT environment. All our developments are made in C++ to provide good performance in our components. The use of COM CAPE-OPEN interfaces was therefore obvious. We include COM definition files directly in our application to respect immediately the interface format. The choice of COM can also be useful to develop Visual Basic script test of components before integration (an example is the CO tester). One of the main risk our project was a possible loss of performance.

**Performance**

- **COM middleware**

After implementation of some CAPE-OPEN components, the use of a COM middleware has no impact on performance, it’s just one more pointer in the system. But the performance of the CAPE-OPEN interface depends on the way you implement it.

- **Information access**
If we go through the CAPE-OPEN interface each time we need to access at one Unit Operation Parameter, this may need more time than a proprietary access. We try to use CAPE-OPEN interfaces in configuration, and not in calculation where all the pointers of the requested objects are stored. The thermodynamic and physical properties document describes static and dynamic properties for calculation that are stored in a Material Object component. The structure of this interface allows for updating of properties without changing CAPE-OPEN interfaces. But we don’t have direct access to properties as in traditional simulation tools. Each time we want to read or write a property, we have to use a map structure with the name of the property. The CAPE-OPEN proposal is an open solution with potential for addititional facilities, but it needs some work to get performance access.

Calculations

In thermodynamic package, all property calculations are called from the MaterialObject interface and executed by the PropertyPackage. The Property Package is not allowed to calculate and store values of properties that have not been specifically requested. Properties cannot be stored in the Material Object, but in the Property Package which can use a cache buffer like processors in hardware architecture, and retrieve property value without any calculation. This approach has been proven to be at least as efficient as traditional approach. However, the CAPE-OPEN property access is not powerfull for iterative calculation – as in a flash solving algorithm. We are working on this subject to improve performance and bypass all named access based mechanisms on Material Object property list. CAPE-OPEN implementation needs new behaviours to retrieve calculation optimization of classical performant tools.

Component development

CAPE-OPEN meets our need to capitalize development on process components. The interface also provides ways to include external component in our thermo system. We need such interface because some clients want to add specific flash algorithm in our systems. They have one algorithm which capitalize their experience from several years. An asset of COM components is the ability to extend interface with proprietary interface to meet specific need. Our application requires specific parameter labels to use Unit Operation. We have a standard way to encapsulate custom Unit Operation, but our CAPE-OPEN Unit Operations are designed and optimized to work with that kind of application.
**Component integration**

CAPE-OPEN is made to use easily custom components. The definition of interfaces like error handling is the only way to make integration with supplier software components. The components are not active like agents, but they will report all non-conformities and why they can’t work as you want. The use of error handling is especially necessary for COSE that use cases may be complex. This part and tools like CO tester are two essential pieces for a good dissemination of CAPE-OPEN component developments.

6. **Expected benefits**

Because of CAPE-OPEN, the market will now have access to robust, reliable, commercial simulators that have standard software component interfaces. There are a number of important consequences for suppliers and consumers in the simulation market. Process industries will be able to enjoy the lower cost and lower maintenance of commercial software, but this will be combined with an abundant flexibility. This combination will allow those companies to predict and manage process performance as never before.

**Benefits for users**

- More flexible process modelling by allowing simulation with software components from multiple sources to be assembled easily in a simulation environment;
- Plug and play integration of imported software components (Thermo, Units, Solvers, niche vendors' software components, etc.) alongside the simulation environment native modules and software components;
- Better work process and environment for team working and / or distance working by using web-based components

**Benefits for vendors & academics**

- Increased usage of CAPE tools in industry thanks to open systems and expanding markets and services for CO components
- Strengthens the position of CO simulation environments
- Reduce development time thanks to the CO architecture
- Easy integration of niche solutions
- Specific Unit Operations, Thermo Systems, Solvers, Kinetic Reaction systems, optimisers etc.
The new collaboration framework is called "co-opetition" as defined by Brandenburger and Nalebuff: "Business is co-operation when it comes to creating a pie and competition when it comes to dividing it up". Plug-and-play capacity will stimulate the market and create new opportunities that could never have happened before. New value nets will be created with one supplier being another supplier's competitor, and at the same time the supplier's complementor, as assembling components from these two sources will provide more than just summing up the two parts by operating them separately.

7. The CO-LaN

In a globalised industry, the processes of creating and maintaining the standard, of promoting its world-wide usage, of certifying standard-compatible process simulation components, and of helping companies and universities develop such components can only be established successfully if supported by an electronic work and education infrastructure. The Global CAPE-OPEN project is therefore setting up a world-wide industry-sponsored virtual network which will be responsible for these tasks beyond the duration of the project itself. The CAPE-OPEN Laboratories Network (CO-LaN) has been created to become the internationally recognised labelling and process management organisation for the CAPE-OPEN standard. The missions of the CO-LaN will be:

- Dissemination: provide solutions and facilities that support a good international information and technology distribution.
- CAPE-OPEN specifications life cycling management: take responsibility for organising the maintenance and evolution of the specifications.
- Labelling delivery responsibility: manage the process as well as the labelling steps. The labelling mission should cover both component licence delivery and the recognition of companies for their approved services.
- Ensure that adapted training modules are developed and available on the market place and complement this by providing public-domain technical information.

CO-LaN is a non-for-profit Society. Its constitutive meeting took place on January 30, 2001 in Rueil-Malmaison, France and was attended by numerous representatives from a wide range of operating companies, software vendors as well as universities. Its legal format and its bylaws
had been previously approved by the Steering Committee of Global CAPE-OPEN where representatives from all partners in the GCO consortium are invited to participate.

Organised as a Society under French law of 1901, it is driven by a Board of Directors which will consist of nine members. Execution of the CO-LaN Board of Directors’ decisions are implemented by an Executive Board of three members, a President, a Secretary and a Treasurer. An Annual General Meeting of members is called to ratify decisions and proposals of the Board of Directors, to decide on the course of the Society, to verify how it is managed and to elect the Co-LaN Directors.

Membership is organised in three groups: group A gathers the industrial users of CAPE software; group B gathers the providers of CAPE software; group C gathers administrations, academic institutions carrying out research activities in the field of CAPE, and other interested parties. Membership fees for each category of membership are defined by the CO-LaN Board of Directors so as to meet the needs of the Society and its members. For example, fees are determined by the group of membership, the membership level, the size and type (commercial, academic, individual) of the members. Membership fees and the definitions of different membership levels are set yearly by the Board of Directors and ratified during the Annual General Meeting of members.

The designed membership and fee scheme gives a balanced representation of all organisations and individuals involved in CAPE activities and supporting the CO-LaN goals.

8. Conclusion

All the above initiatives aim at facilitating the widespread adoption of component software as the software technology of the next decade. The small steps that we are taking now (e.g. with CAPE-OPEN) form the foundations of a new wave which will turn the software industry into an industry of reusable components that can be mixed and matched in infinitely various ways. After generations of software technology, from machine code and assembly language through FORTRAN and structured programming to objects, it is now time to embark into this new generation, triggered by the growing demands of millions of users and by the communication needs through the Internet.
Open software architectures are the way forward for the next generation of CAPE tools. They allow previously incompatible environments to inter-operate through commonly agreed interface standards established on top of middleware platforms such as COM and CORBA. Moreover, open software architectures will be the technical basis allowing the sharing between organisations, departments within organisations, and individuals within departments.

The adoption of the CAPE-OPEN standards by a large number of software component is perceived as a way of extending the use of modelling software, which, in turn, should provide a competitive advantage to end users, and providers.

9. References

www.colan.org CAPE-OPEN Laboratories Network web portal
www.global-cape-open.org, Global CAPE-OPEN web site