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CAPE-OPEN Update

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Issue n°05

A compilation of CAPE-OPEN related papers

A compilation of abstracts of papers presented and published regarding the CAPE-OPEN (CO) concepts, the CO standard, Global CAPE-OPEN (GCO) results, the CAPE-OPEN Laboratory Network (CO-LaN), and related topics

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CO-LaN

www.colan.org

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CAPE-OPEN Update is a publication of the **GCO-Support** project in collaboration with the **CO-LaN**, a non-profit consortium for the development of the **CAPE-OPEN** standard.
GCO-Support is funded by the European Community under the «Industrial and Materials Technologies» and «Competitive and Sustainable Growth» Programmes.

1999

IST99 Helsinki: Information Society Technologies Conference, Helsinki, November, 1999 www.ist99.fi. http://europa.eu.int/comm/information_society/ist/conference_en.htm,

Global CAPE-OPEN: Delivering The Power of Component Software and Open Standard Interfaces in Computer-Aided Process Engineering

Bertrand BRAUNSCHWEIG **Institut Français du Pétrole**

Abstract:

In this paper, we present an international initiative in open software architecture for Computer-Aided Process Engineering (CAPE): Global CAPE-OPEN, an IMS proposal that builds on the result of the EC-funded CAPE-OPEN project. We look at the key industrial issues in the sectors addressed; we present the project technology and the expected benefits of using this technology; we present the achievements until today, mainly from the CAPE-OPEN project; we assess the benefits of international co-operation on this subject; we finish by looking at possible future directions for research and development in this area. We conclude with some remarks on the project management in relation with the IMS organisation.

2000

AIChE Spring Meeting, Atlanta, Georgia, USA, March 2000 (American Institute of Chemical Engineers).

Global CAPE-OPEN: Delivering The Power of Component Software and Open Standard Interfaces in Computer-Aided Process Engineering

Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

Computer Aided Process Engineering (CAPE) is now required to be competitive in the Chemical Process Industries (CPI). An international initiative is underway to develop and implement open software architecture standards: Global CAPE-OPEN, an Intelligent Manufacturing Systems (IMS) project that builds on the result of the EC-funded CAPE-OPEN project. This paper looks at the relevant key issues in the CPI, CAPE-OPEN technology and the expected benefits of using this technology, progress to date in CAPE-OPEN and Global CAPE-OPEN, the benefits of international co-operation; and directions for research and development in this area.

2001

Article in CAST, the AIChE journal of the Computing and Systems Technology group. Spring 2001. http://www.castdiv.org/ArchivedNewsletters.htm

Global CAPE-OPEN: Delivering the power of component software and open standard interfaces in Computer-Aided Process Engineering

Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

Chemical manufacturers typically employ a collection of software (in-house, commercial, and/or academic) to solve various CAPE-related problems. Before solving such problems, it should be possible for the process engineer to 'assemble' the necessary computational tools with the minimum effort. The objective of the Global CAPE-OPEN (GCO, http://www.global-cape-open.org) project is to deliver the power of component software and open standard interfaces in computer-aided process engineering. The CAPE-OPEN project established a set of standards (http://www.global-cape-open.org/CAPE-OPEN_standard.html) to allow communication between various pieces of software from different sources (software and equipment vendors, universities, and company generated). GCO uses CO results and capitalises on further opportunities that can be gained from open standard interfaces for process simulation.

GCO addresses and answers the following questions:

- How will open process simulation technology be integrated into the process engineering work process?
- How can industry take better advantage of open architectures and standards?
- What are the other open standard interfaces needed for CAPE?
- How is CAPE-OPEN compliant software to be developed?
- How will CAPE-OPEN compliant components be certified and labelled as such?

A consortium representing a wide range of users, researchers and vendors from three continents is answering these questions by developing what can be considered as the second stage of the CAPE-OPEN initiative.

This will provide the process industries with faster, cheaper, more accurate process simulation leading to enhanced competitive and environmental performance. A large new market will be created for specialist simulation vendors, increasing competition and advancing the state-of-the-art.

The GCO project will:

- Develop additional open standard interfaces for CAPE components
- Adapt existing software so that it complies with the CO standard
- Develop methods, training and support tools for helping users to take advantage of the availability of CO-compliant components.

In the course of the project, the consortium will launch «CO-LaN», the CAPE-OPEN Laboratories Network, which will be open to other organisations worldwide, and will manage all aspects of the CAPE-OPEN standards and certification on a long-term basis

ESCAPE 11 Conference, Kolding, Denmark, May 2001. Available in Computer-Aided Chemical Engineering, 9, Elsevier, Editors R. Gani & S.B. Jorgensen pp 967-972, 2001.
http://www.elsevier.nl

Open Software Architectrue for Numerical Solvers: Design, Implementation and Validation

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Laboratoire de Génie Chimique CNRS INPT-ENSIACET

Introduction

Traditional simulation environments are closed monolithic systems. The resulting bottlenecks in interoperability, reuse and innovation led to the CAPE-OPEN and the GLOBAL-CAPE-OPEN projects2, in which the chemical and oil industries, academics and software suppliers are defining standards for a component-based approach to process simulation. The resulting standard, CAPE-OPEN (CO) [1] [2], is now widely disseminated. This standard distinguishes two kinds of software components: Process Modelling Components (PMC) and Process Modelling Environments (PME). Its current version defines several PMC interfaces such as the CO Numerical Solver.

In this paper, we first discuss on the CO Numerical Solvers specification and design. Then, we give an overview and a feedback on Numerical Services Provider (NSP). Finally, some process applications using the NSP are considered.

CO Numerical Solvers : Analysis, design and specification

An upper abstraction level defines four packages where the interfaces are specified. A) The Solver package 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 and sparse systems of linear algebraic equations (LAE), non linear algebraic equations (NLE) and mixed differential and algebraic equations (DAE). B) The Eso package contains the Equation Set Object (ESO) concept which is an abstraction representing a square or rectangular set of equations. Those equations define the physical behaviour of the process under consideration. An ESO is a purely continuous mathematical description: the equations remain the same for all the possible values of the variables. C) The Model package introduces the Model object to embody the general mathematical description of a physical system. The fundamental building block employed for this purpose is a set of ESO. However, many physical systems also involve discontinuities, and this fact must be reflected in their mathematical description. Accordingly, a Model may additionally encompass one or more State Transition Networks (STN) [3]. These are formal descriptions of discontinuous phenomena. D) The Utility package has the Parameter concept that allows some customisation of each component. Nevertheless this gain in flexibility leads to a reduction of standardisation capability.

This set of specifications incorporates the CO architecture that leans on the distributed component (heterogeneous) system and the object-oriented paradigm. The involved technologies are the UML notation [4], the CORBA [5] and (D)COM [6] middleware, the CO Work Process and object-oriented languages.

The limits of the CO Numerical Solvers, version 0.9, are discussed and some ways for improvement are proposed.

Numerical Services Provider (NSP) : Implementation

The implementation of the full CO Numerical Solvers is a PMC called NSP. According to the component scheme, it realises the Solver component depending on the Model and Eso components. Following the CO architecture for CORBA, NSP acts as a numerical server through the object request broker and employs the common services as well as an error handling strategy. It stands for the second stage (that is to say the business model) within the 3-tiers architecture. Obviously, this stage is a separate process that can be used on a single machine, or across the network within an internet-based enterprise business system.

NSP combines Java and C++ codes as well as Fortran 77 legacy codes. Within a specific hierarchy it supplies the LAE, NLAE and DAE objects, jointly to configuration parameter objects. These solvers come from research work on dynamic simulation of hybrid systems [7]; their new capabilities are detailed.

The limits of this application are discussed and some future improvements are introduced.

Applications using the NSP : Validation

Several PME applications that are compliant with the CO Numerical Solvers use the NSP in order to solve their process mathematical model. They rely on the CO architecture for CORBA; especially they comply with the bind process, the error handling strategy and the interworking recommendations for COM based applications. They correspond to the first stage and have to provide the Model and the Eso components to the NSP. Some process are simulated taking advantage of the following PME: a State Machine Builder prototype, which solves hybrid and dynamic systems and environments coming from different software suppliers.

Conclusion

Open software architectures are the way forward for the next generation of CAPE tools. The CO standard achieves true plug and play of industry business components in enterprise software. The current CO Numerical Solvers specification is set out and discussed. The first complete implementation of this standard leads to the NSP application that provides numerical services to several CO compliant PME. Its realisation validates not only the business interfaces but also the overall architecture for a CO process simulation.

ICheaP-5 (Italian Conference on Chemical and Process Engineering), Florence, Italy, May 2001, AIDIC Conference Series, Elsevier Editoriale Italia, Vol. V, 2001.
http://www.aidic.it/italiano/congressi/icheap5/

A Virtual Organisation for Managing CAPE-OPEN (CO) Standards

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG and Pascal ROUX — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Jörg KÖLLER and Alexander KUCKELBERG — **RWTH Aachen Informatik V**

Abstract:

A standardisation body (CAPE-OPEN Laboratories Network - CO-LaN) has been established early in 2001 to maintain and disseminate the software standards in the Computer Aided Process Engineering (CAPE) domain that have been developed in the international projects CAPE-OPEN and Global CAPE-OPEN. CO-LaN ensures that software tools used by the process industries reach a level of interoperability that will help ensure sustained growth and competitiveness. Missions of CO-LaN include managing the life cycle of the published standards, dissemination about CAPE-OPEN standards and compliance checking of software components implementing these standards as well as maintaining a dictionary of all existing CO software components. A number of advanced tools have been and will be developed to sustain such missions, giving sound reasons for joining the CO-LaN which is providing numerous services to its members as well as to the CAPE community at large.

ICheaP-5 (Italian Conference on Chemical and Process Engineering), Florence, Italy, May 2001, AIDIC Conference Series, Elsevier Editoriale Italia, Vol. V, 2001.
http://www.aidic.it/italiano/congressi/icheap5/

Global CAPE-OPEN (GCO) project results to date: May 2001

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

Manufacturers in the process industries must use a collection of software (in-house, commercial, and/or academic) to perform Computer Aided Process Engineering (CAPE) because the market for process simulation has been so far one of incompatible proprietary products. More effective CAPE is required to be competitive in the process industries. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to insure interoperability of CAPE software components. Results of the GCO project to date include new common and dedicated CAPE-OPEN interface specifications, CO compliant software components and modelling environments, prototypes, organisations as well as new advanced concepts.

ECCE3 (3rd European Congress of Chemical Engineering) conference, Nuremberg, Germany, June 2001. http://sun.vdi-online.de/gvc/ecce/

CAPE-OPEN (CO) standards: implementation and maintenance

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG and Pascal ROUX — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Jörg KÖLLER and Alexander KUCKELBERG — **RWTH Aachen**

Abstract:

A standardisation body (CAPE-OPEN Laboratories Network - CO-LaN) has been established to maintain and disseminate the software standards in the Computer Aided Process Engineering (CAPE) domain that have been developed in the international projects CAPE-OPEN and Global CAPE-OPEN. The CO-LaN ensures that software tools used by the process industries reach a level of interoperability that will help ensure sustained growth and competitiveness. Goals and means of the CO-LaN are described, especially its work process related to testing procedures applied to software components in order to assess their compliance with the published CAPE-OPEN interface specifications.

ECCE3 (3rd European Congress of Chemical Engineering) conference, Nuremberg, Germany, June 2001. http://sun.vdi-online.de/gvc/ecce/

Global CAPE-OPEN (GCO) project results to date: June 2001

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

Manufacturers in the process industries must use a collection of software (in-house, commercial, and/or academic) to perform Computer Aided Process Engineering (CAPE) because the market for process simulation has been so far one of incompatible proprietary products. More effective CAPE is required to be competitive in the process industries. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to insure interoperability of CAPE software components. This paper presents results of the GCO project to date.

6th World Congress of Chemical Engineering, Melbourne, Australia, September 2001.
http://www.chemengcongress.com/

Global CAPE-OPEN (GCO) project results to date

Rafiql GANI — **Denmark Technical University**
Peter MAUER — **BASF**
Michel PONS — **ATOFINA**
Kerry IRONS and Werner MERK — **The Dow Chemical Company**
Peter BANKS — **BP International Ltd.**
Pascal ROUX — **Institut Français du Pétrole**
Knut MATHISEN — **Norsk Hydro**

Abstract:

Manufacturers in the process industries must use a collection of software (in-house, commercial, and/or academic) to perform Computer Aided Process Engineering (CAPE) because the market for process simulation has been so far one of incompatible proprietary products. More effective CAPE is required to be competitive in the process industries. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to insure interoperability of CAPE software components. Results of the GCO project to date include new common and dedicated CAPE-OPEN interface specifications, CO compliant software components and modelling environments, prototypes, a web site for information and education, a means to label CO compliant software components, software component testers, organisations, and new advanced CAPE concepts.

6th World Congress of Chemical Engineering, Melbourne, Australia, September 2001.
http://www.chemengcongress.com/

CO-LaN: Maintaining the CAPE-OPEN standard through a virtual organisation

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHEIGand Pascal ROUX — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Jörg KÖLLER and Alexander KUCKELBERG — **RWTH Aachen**

Abstract:

Process Industry companies must use a collection of software to perform Computer Aided Process Engineering (CAPE) tasks since the market for process simulation has been so far one of incompatible proprietary products. The CAPE-OPEN (CO) project established a set of standards to allow communication between software from different sources (software and equipment vendors, universities, and «home grown»). Global CAPE-OPEN (GCO) is an Intelligent Manufacturing Systems (IMS) project that builds on the results of CAPE-OPEN. GCO is leading to the global acceptance of CO standards. Upon GCO completion, the CAPE-OPEN Laboratories Network (CO-LaN) will serve to perpetuate the CO interface standards. The general goals of the CO-LaN are to provide a means to label CO compliant software components, to insure maintenance and addition of needed interface standards, and to ensure the implementation of the CO interface standards in the CAPE community. The CO-LaN is operating during the GCO project both to establish itself as the labelling and testing body for CO and to offer a way for organisations who are not members of GCO to become involved in the project.

SIIT (Standardisation & Innovation in Information Technology) Conference Boulder, Colorado, USA, October 2001. http://www.siit2001.org/

CAPE-OPEN (CO) standards: implementation and maintenance

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Jörg KÖLLER and Alexander KUCKELBERG — **RWTH Aachen**

Abstract:

A standardisation body (CAPE-OPEN Laboratories Network) has been established to maintain and disseminate the software standards for Computer Aided Process Engineering (CAPE) domain developed in the international projects CAPE-OPEN and Global CAPE-OPEN. It ensures that software tools used by most Process Industries reach a level of interoperability required for sustained growth and competitiveness. Goals and means of this body are described as well as some parts of its work process, especially related to the development of standards specifications.

It is well established that some form of simulation is a major activity in the synthesis, design, operation/control, and planning of a process within any chemical company. Process simulation allows the engineer to study and assess process alternatives with respect to economic, safety, and environmental performance without actually building a plant, thereby reducing cost and speeding up the design of the plant. Simulation programs can be used for various purposes in nearly every development stage of a chemical plant [1, 2, 3].

Information about equipment design parameters, specification of design parameters, mathematical models for unit operations, etc. is needed before a simulation can be performed. Unfortunately, the information and models are distributed over multiple isolated Computer Aided Process Engineering (CAPE) tools having individual strengths and weaknesses. Hence chemical manufacturers must use a collection of software (in-house, commercial, and/or academic) to perform CAPE tasks - the market for process simulation has been one of incompatible proprietary products, with manual transfer of data and models. Obviously this is expensive and error-prone.

A solution to this problem is the design of open and standardised interfaces facilitating the integration of external modules contained in other tools, or independently developed for a specific purpose. Open interfaces allow direct exchange of data between different applications. For process simulators, this problem was addressed and solved by the CAPE-OPEN initiative [4]. The design of such open interfaces has a practical use and will enhance the quality of process simulators.

SIIT (Standardisation & Innovation in Information Technology) Conference Boulder, Colorado, USA, October 2001. http://www.siit2001.org/

Research Efforts in Computer-Aided Process Engineering/ Open Architecture (CAPE-OPEN)

Kerry IRONS — **The Dow Chemical Company**
Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG and Pascal ROUX — **Institut Français du Pétrole**
Knut Wiig Mathisen — **Norsk Hydro**
Rafiqul Gani, — **Denmark Technical University**

Abstract:

The objective of the Global CAPE-OPEN (GCO) project is to deliver the power of component software and open standard interfaces in computer-aided process engineering. GCO capitalises on opportunities that can be gained from open standard interfaces for process simulation. GCO has a number of aspects, but includes a significant research component. The research thrusts and results of GCO are summarised in this review of the project.

International IMS (Intelligent Manufacturing Systems) Project Forum 2001, CO-LaN Concept Review - October 2001. http://www.cimsi.cim.ch/IMS_Forum_2001/

The CAPE-OPEN Laboratories Network. An IMS project gives birth to a non-profit neutral industry and academic association

Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Michel PONS — **ATOFINA**

Abstract:

The EU-project CAPE-OPEN (CO) has defined a component based software standard to overcome the bottlenecks in interoperability and innovation of simulation software by assuring plug-and-play interoperability of components offered by various vendors. One of the goals and achievements of the follow-up EU/IMS-project Global CAPE-OPEN (GCO) is the installation of a membership-based organisation called the CAPE-OPEN Laboratories Network (CO-LaN), responsible for dissemination and maintenance of the CO standard.

CO-LaN is non-profit neutral industry and academic association promoting open standards in process simulation software. CO-LaN members are committed to making Computer Aided Process Engineering (CAPE) easier, faster and less expensive by achieving complete interoperability of CAPE-OPEN compliant commercial CAPE software tools.

Testing procedures and software will be publicly available both for development and labelling purposes. A dictionary, maintained by the CO-LaN and containing detailed product information on labelled components, will help end-users finding the products they need. Additionally, the CO standard facilitates new business models for process simulation software such as various application service provider approaches.

The paper presents the results of CAPE-OPEN, Global CAPE-OPEN, and the missions and technical infrastructure of the CO-LaN.

European Commission's IST Programme's e2001 - The eBusiness and eWork conference, October 2001 Venice, Italy. http://www.dlr.de/e2001/e2001brokerage/e2001welcome.htm
Proceedings: E-work and E-commerce: «Novel Solutions and Practices for a Global Networked Economy» from http://www.amazon.co.uk

The CAPE-OPEN Laboratories Network: Standards for Interoperable Process Engineering Software Components

Mathias JARKE and Jörg KÖLLER — **RWTH Aachen**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**
Michel PONS — **ATOFINA**

Abstract:

Facing economic, environmental, and safety constraints, the process industries (chemicals, oil and gas, food) are forced to improve performance of their plants and to reduce time for product development phases and innovation cycles. Process simulation has become a vital tool in order to achieve these goals. Despite of this market pressure, valuable research results find their way only slowly into commercial process simulation software, because until now these systems were not interoperable.

The EU-project CAPE-OPEN (CO) has defined a component based software standard to overcome the bottlenecks in interoperability and innovation of simulation software by assuring plug-and-play interoperability of components offered by various vendors. One of the goals and achievements of the follow-up EU-project Global CAPE-OPEN (GCO) is the installation of a membership-based organisation called the CAPE-OPEN Laboratories Network (CO-LaN), responsible for dissemination and maintenance of the CO standard. The CO-LaN offers to visitors and member various web-based services in a web-portal targeted at supporting and bringing together suppliers and users of simulation software. The CO-LaN is responsible for labelling software components as CO compliant.

The process simulation market is led by a few major vendors. SME's providing specialised process simulation components will easily enter the market through the CO-LaN. A potential of approximately 2000 companies acting as component suppliers is envisioned on this marketplace.

Testing procedures and software will be publicly available both for development and labelling purposes. A dictionary, maintained by the CO-LaN and containing detailed product information on labelled components, will help end-users finding the products they need.

Additionally, the CO standard facilitates new business models for process simulation software such as various application service provider (ASP) approaches.. As the major simulation software vendors already offer commercial products implementing the CO standard, smaller companies are likely to follow, helped by the CO-LaN infrastructure.

GP2001 conference (8ème congrès Francophone de Génie des Procédés. Organised by SFGP (Société Française de Génie des Procédés)), Nancy, October 2001. Proceedings in Récents progrès en génie des procédés N°82 Vol.15 2001: information, modélisation, simulation et optimisation, Editors(s) : Latifi A., Boudrant J., Tondeur D., 512 p. Can be purchased from Lavoisier, http://www.lavoisier.fr/

Global CAPE-OPEN (GCO) project results to date: June 2001

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

Manufacturers in the process industries must use a collection of software (in-house, commercial, and/or academic) to perform Computer Aided Process Engineering (CAPE) because the market for process simulation has been so far one of incompatible proprietary products. More effective CAPE is required to be competitive in the process industries. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to insure interoperability of CAPE software components. This paper presents results of the GCO project to date.

GP2001 conference (8ème congrès Francophone de Génie des Procédés. Organised by SFGP (Société Française de Génie des Procédés)), Nancy, October 2001. Proceedings in Récents progrès en génie des procédés N°82 Vol.15 2001: information, modélisation, simulation et optimisation, Editors(s) : Latifi A., Boudrant J., Tondeur D., 512 p. Can be purchased from Lavoisier, http://www.lavoisier.fr/

CO-LAN: Missions and means of the CAPE-OPEN Laboratories Network

Michel PONS — **ATOFINA**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Kerry IRONS — **The Dow Chemical Company**

Abstract:

A standardisation body (CAPE-OPEN Laboratories Network - CO-LaN) has been established early in 2001 to maintain and disseminate the software standards in the Computer Aided Process Engineering (CAPE) domain that have been developed in the international projects CAPE-OPEN and Global CAPE-OPEN. CO-LaN ensures that software tools used by the process industries reach a level of interoperability that will help ensure sustained growth and competitiveness. Missions of CO-LaN include managing the life cycle of the published standards, dissemination about CAPE-OPEN standards and compliance labelling of software components implementing these standards. A number of advanced tools have been and will be developed to sustain such missions, giving sound reasons for joining the CO-LaN which is providing numerous services to its members as well as to the CAPE community at large.

AIChE Annual Meeting (American Institute of Chemical Engineers), Reno, Nevada, USA, November 2001.

New Generation Simulation Environment: Technical Vision of the CAPE-OPEN Standard

Jean-Pierre BELAUD, — **Laboratoire de Génie Chimique CNRS INPT-ENSIACET**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Michel PONS — **ATOFINA**
Kerry IRONS — **The Dow Chemical Company**
Michael HALLORAN and Daniel PIÑOL — **Aspen Technology Inc.**

Abstract:

Open software architectures are the way forward for the next generation of CAPE (Computer Aided Process Engineering) tools [BRAUNSCHWEIGet al., 1999]. The CAPE-OPEN (CO) standard achieves true plug and play of process industry simulation software components. Traditional simulation environments are closed monolithic systems; and the resulting bottlenecks in interoperability, reuse and innovation have led to the CAPE-OPEN and GLOBAL-CAPE-OPEN projects. These projects represent a collaboration between the chemical and petroleum refining industries, academics, and software suppliers; with a view to defining a standard for component-based approach to process simulation.

We will focus on the technology associated with the CO standard within the framework of the current version (0.9.3). In order to illustrate this technical vision, we will show two commercial software components that are compliant with the CO standard. Finally we will give an overview of future development actions that will distribute to the CAPE community a standard that is ever more reliable, comprehensive and complete.

The CAPE-OPEN standard results from the CAPE-OPEN and GLOBAL CAPE-OPEN projects and has begun to be widely disseminated to the chemical engineering community. CAPE-OPEN project was funded under the EU Brite EuRam framework, and Global CAPE-OPEN project is funded by the European Community under the «Industrial and Materials Technologies» and «Competitive and Sustainable Growth» Programmes. In addition, Global CAPE-OPEN project follows the Intelligent Manufacturing Systems initiative promoting collaboration between six international regions. The CO-LaN consortium [CO-LaN, 2001] is now in charge of managing lifecycle. This non-for profit organisation maintains the CO standard, disseminates about the standard and labels software components as CO compliant. With more than 20 members (operating companies, vendors and academics) it provides a service to the CAPE community in all aspects of CO standard.

AIChE Annual Meeting (American Institute of Chemical Engineers), Reno, Nevada, USA, November 2001.

GLOBAL CAPE-OPEN (GCO) project results to date

Rafiq GANI — **Denmark Technical University**
Peter MAUER — **BASF**
Michel PONS — **ATOFINA**
Kerry IRONS — **The Dow Chemical Company**
Peter BANKS — **BP International Ltd.**
Bertrand BRAUNSCHWEIG and Pascal ROUX — **Institut Français du Pétrole**
Knut MATHISEN — **Norsk Hydro**

Abstract:

Manufacturers in the process industries must use a collection of software (in-house, commercial, and/or academic) to perform Computer Aided Process Engineering (CAPE) because the market for process simulation has been so far one of incompatible proprietary products. More effective CAPE is required to be competitive in the process industries. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to insure interoperability of CAPE software components. Results of the GCO project to date include new common and dedicated CAPE-OPEN interface specifications, CO compliant software components and modelling environments, prototypes, a web site for information and education, a means to test CO compliant software components, software component testers, organisations, and new advanced CAPE concepts.

2002

IChemE (Institute of Chemical Engineers) Subgroup on CAPE, Cranfield, UK. March, 2002.
http://www.icheme.org/

CFD - Tool or Toy? - The Role of CFD in Computer-Aided Process Engineering

C. CAREY **Fluent Europe**

Abstract:

The U.S. Dept. of Energy (DOE) Vision 21 programme aims to meet the long-term demands of the U.S. economy for fossil-fuel based commodities. These range from steam, electricity and motor fuels to hydrogen, syngas and chemicals. The power plants that produce them need to be flexible, modular, and to achieve unprecedented increases in efficiency and environmental performance. The target is to have such plants up and running in 15 years.

DOE plan to reduce the time and cost of development by using simulation. To do so, they need to seamlessly link computer models that represent individual plant modules such as boilers, gasifiers, fuel cells and turbines. The first step towards providing this «virtual simulation» capability is described. The demonstrator links the Aspen Plus process simulation package from Aspen technology with the FLUENT CFD package from Fluent Inc. to model a reaction-separation-recycle flowsheet that includes a CSTR. This allows you to investigate how yield and purity of the CSTR product vary with agitator design and speed.

Integration is achieved using:

(1) Global CAPE-OPEN Interfaces for unit operations thermodynamics and reaction kinetics. These allow:
- the use of FLUENT CDF models in an Aspen Plus flowsheet
- exchange of stream information between the two
- transfer of Aspen Plus physical property and kinetic data to FLUENT

(2) A COM-CORBA bridge that allows Aspen Plus and FLUENT to run on different hardware platforms and under different operating systems.

ESCAPE 12 conference, Delft, Netherlands, May 2002. Available in Computer-Aided Chemical Engineering, 10, Elsevier, pp 847-852, 2002. Editors J. Grievink, J. van Schijndel.
http://www.elsevier.nl

Open Software Architecture For Process Simulation: The Current Status of CAPE-OPEN Standard

Jean-Pierre BELAUD — **Laboratoire de Génie Chimique CNRS INPT-ENSIACET**
Michel PONS — **ATOFINA**

Abstract:

Traditionally simulation environments have been closed monolithic systems and the resulting bottlenecks in interoperability, reuse and innovation have led to the search for a more open and interoperable solution. The CAPE-OPEN (CO) effort, launched in January 1997, is a standardisation process for achieving true plug and play of process industry simulation software components. The resulting CO standard is now being widely disseminated to the chemical engineering community. It relies on a technology that integrates up to date concepts from the software field such as a component-based approach. A number of software components based on this technology have been developed and are already available. Thanks to this new generation of CAPE tools, it is expected to reach cheaper, better and faster design, operation and control of processes. The CAPE-OPEN Laboratories Network (CO-LaN) consortium is in charge of managing the lifecycle of the CO standard.

ESCAPE 12 conference, Delft, Netherlands, May 2002. Available in Computer-Aided Chemical Engineering, 10, Elsevier, pp 853-858, 2002. Editors J. Grievink, J. van Schijndel.
http://www.elsevier.nl

An Open Software Architecture for Steady-Sate Data Reconciliation and Parameter Estimation

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Universitat Politècnica de Catalunya, Chemical Engineering Department

Abstract:

In this paper a flexible and open architecture design for Parameter Estimation and Data Reconciliation (PEDR) software application is proposed by de-coupling it according to the functionalities involved. In the proposed approach the different components that are involved in this application and their interactions are specified and tested. The proposed architecture aims at an improved efficiency and upgrading of the PEDR application by allowing the exchangeability and connectivity of the present components in an easy and consistent way.

ESCAPE 12 conference, Delft, Netherlands, May 2002. Available in Computer-Aided Chemical Engineering, 10, Elsevier, pp 919-924, 2002. Editors J. Grievink, J. van Schijndel.
http://www.elsevier.nl

Nonlinear Analysis of gPROMS Models using DIVA via a CAPE ESO Interface

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Abstract:

The CAPE ESO interface of the process simulator gPROMS is used to pass model information to numerical methods contained in the simulation environment DIVA. By the interface, algorithms for the continuation of stable and unstable steady state and periodic solutions can be applied directly to gPROMS models. The use of the interface is illustrated by a detailed nonlinear model of an industrial reactive distillation column.

ESCAPE 12 conference, Delft, Netherlands, May 2002. Available in Computer-Aided Chemical Engineering, 10, Elsevier, pp. 859-864, 2002. Editors J. Grievink, J. van Schijndel.
http://www.elsevier.nl

TRIZ and the evolution of CAPE tools From FLOWTRAN® to CAPE-OPEN® and beyond

Bertrand BRAUNSCHWEIG Institut Français du Pétrole
Kerry IRONS The Dow Chemical Company

Abstract:

The paper looks at trends in evolution of software tools with a particular emphasis on CAPE applications. Using results from TRIZ (Theory of Inventive Problem Solving), we show why and how CAPE software follows a major trend towards distributed adaptive heterogeneous components. Consequently, and thanks to the CAPE-OPEN communication infrastructure, we show that CAPE models can be made of distributed autonomous agents that we nickname «cogents».

ESCAPE 12 conference, Delft, Netherlands, May 2002 Included in the previous article and available in Computer-Aided Chemical Engineering, 10, Elsevier, pp 859-864, 2002. Editors J. Grievink, J. van Schijndel. http://www.elsevier.nl

COGents: a new IST-funded project on CAPE-OPEN Software Agents

Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Eric S. FRAGA — **Department of Chemical Engineering, University College London**
Zahia GUESSOUM — **OASIS group**
Didier PAEN — **R.S.I**
Daniel PIÑOL — **Aspen Technology Inc.**
Aidong YANG — **RWTH Lehrstuhl für ProzessTechnik**

Abstract:

COGents is a EC-funded IST project aimed at developing an agent-based architecture for numerical simulation, with a concrete implementation in the process simulation domain relying on the CAPE-OPEN interoperability standard. The COGents architecture will enable innovative application service provision in numerical simulation. The project, which lasts two years (April 2002-March 2004), will propose and implement a framework, will design the OntoCAPE domain ontology of modelling knowledge, and will demonstrate its business benefits through two realistic case studies.

COGents is funded by the European Community under the Information Society Technologies programme, contract IST-2001-34431.

15th CHISA conference (International Congress of Chemical and Process Engineering), Prague, Czech Republic, August 2002. http://www.chisa.cz/2002/

Open Bed-Reactor Modelling Software Component

Jean Pierre BELAUD — **Laboratoire de Génie Chimique CNRS INPT - ENSIACET**
Michel PONS — **ATOFINA**
Pascal ROUX — **Institut Français du Pétrole**

Abstract:

Open software architectures are the way forward for the next generation of CAPE (Computer Aided Process Engineering) tools. The CAPE-OPEN (CO) standard achieves true plug and play of process industry simulation software components. Traditional simulation environments are closed monolithic systems; and the resulting bottlenecks in interoperability, reuse and innovation have led to the CAPE-OPEN and Global CAPE-OPEN projects. These projects represent a wide collaboration between the chemical and petroleum refining industries, academics, and software suppliers; with the goal of defining a standard for a component-based approach to process simulation. The resulting standard, CAPE-OPEN, is now widely disseminated in the chemical engineering community. The CO-LaN consortium is in charge of managing its lifecycle. With

more than 20 members (operating companies, software suppliers and academics) it provides services to the CAPE community in all aspects of CO standards.

This paper focuses on the solutions provided by the CAPE-OPEN standard for unit operations. They rely on the distributed component (heterogeneous) system and the object-oriented paradigm. The involved software technologies are the UML notation, the web enabled CORBA and (D)COM middleware, and the Unified Processes and object-oriented programming languages.

We first introduce the CO Unit Operation specification and design. Then, we present a CO compliant bed reactor model developed by Institut Français du Pétrole. Finally, process applications using this unit operation component are considered.

The CO standard defines a comprehensive set of standard interfaces for unit operation modules being used within modular and steady-state simulation environments. 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. A material Port is associated with a Material Object. Ports also have 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. 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).

Within this scope, we have selected a real case of a reactor model that has industrial relevance such as MTBE or isooctane production as shown in figure 1.

The CO reactor component includes COM objects that use and implement the appropriate CO interfaces, a graphical user interface, a wrapper layer and a FORTRAN 77 calculation engine. This engine provides kinetic, thermodynamic, hydrodynamic and numerical computations.

Thus, this reactor can be plugged into any simulation environment that is compliant with CO architecture for Unit Operation. For example, the Institut Français du Pétrole reactor component is integrated into the HYSYS.Process environment from Hyprotech for solving a specific flowsheet as illustrated in figure 2.

The CO standard delivers to process engineers more flexible process modelling tools by allowing simulation with software components from multiple sources, assembled easily in widely used simulation environments. It is no longer necessary to comply with procedures specific to each environment in order to run in-house unit operations. Develop once, design and simulate everywhere, as a CO compliant unit operation software component such as the Institut Français du Pétrole reactor can now be integrated in any CO compliant environment through simple «plug and play» operations. The CO standard benefits software component developers by increasing the usage of CAPE tools and by reducing the development cost. It also extends for each simulation environment the tool set that can be selected by process simulation engineers.

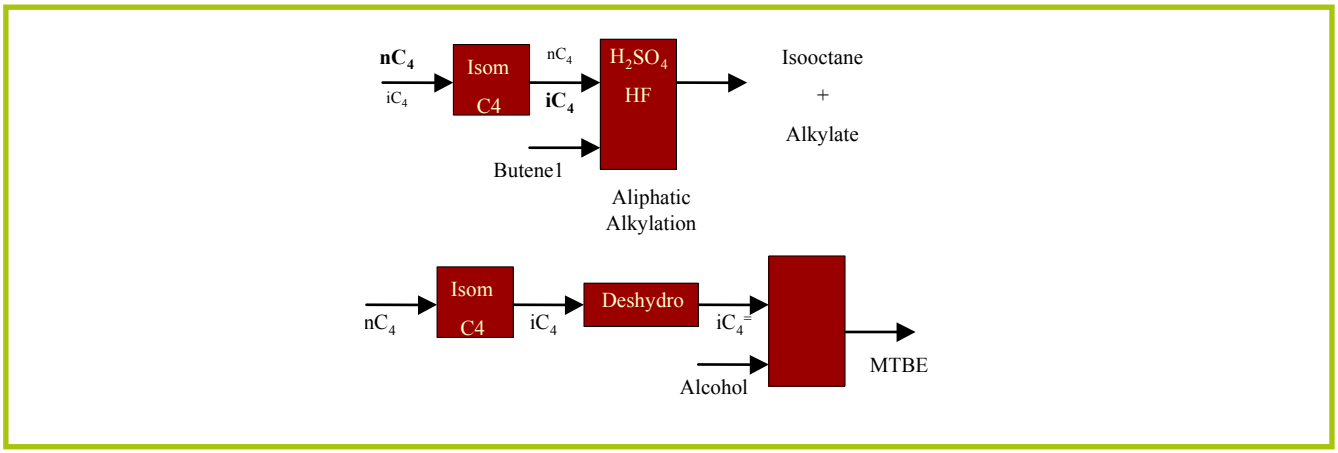

Figure 1 : Industrial Applications

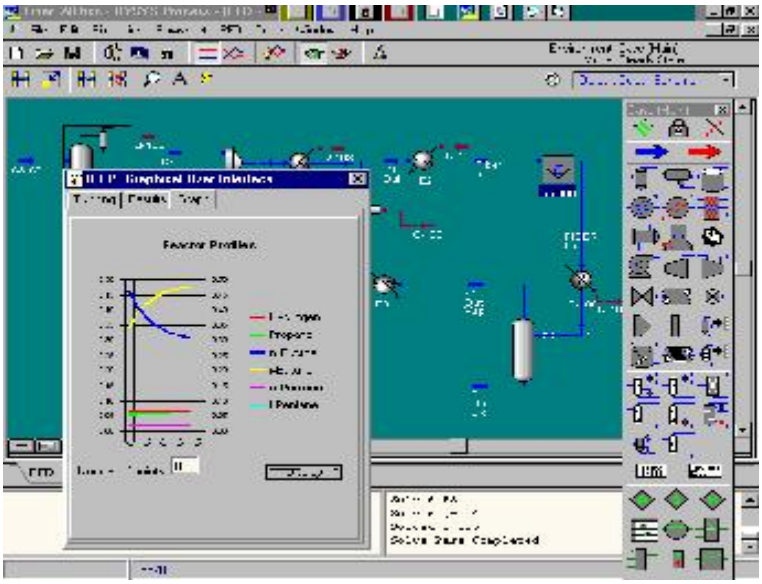

Figure 2 : Process Simulations

ECTP 2002, 16th European Conference on Thermophysical Properties, Imperial College, London, September 2002. For a CD ROM of the proceedings: conference@npl.co.uk, (National Physical Laboratory, Teddington, Middlesex, UK, TW11 0LW.)

The CAPE-OPEN interface specification for Physical Properties Databanks

Michel PONS **ATOFINA**

Abstract:

Pure and mixture physical property data are necessary in the chemical process industries for a number of purposes which are most often related to the modelling, simulation and control of production processes: process synthesis, process simulation, plant optimisation and production control are typically some of the domains concerned with the use of models in which pure and mixture physical property data are embedded or accessed from suitable data banks.

In the process simulation domain, software tools such as PRO/II , Hysys.Process or AspenPlus , are extremely valuable to the process engineer: they have emerged as standard tools on any process engineer desk. But each of them cannot cover the entire range of tasks a process engineer has to fulfill. So a process engineer needs to use several software tools supplied by different vendors, for example to carry on a single project.

In the past, each computer program used its own data bank which could not be accessed from any third party software. So the consistency of data throughout the process engineering workflow was not supported. A few programs allowed the user to specify its own data sets, but most of them used different formats, preventing a convenient sharing of information.

On the other hand, large commercial data bases containing thermophysical property data have evolved in the last two decades. Organisations like DIPPR in the USA and DECHEMA in Germany have established

links between their data banks and process simulation programs. But each link represents a specific piece of work.

From July 1999 till March 2002, the Global CAPE-OPEN (GCO) consortium involved a wide range of leading process industry companies, researchers, and software vendors in Europe, Asia, and North America. The objective of the GCO project was to deliver the power of component software and open standard interfaces in computer-aided process engineering. GCO used CAPE-OPEN (CO) results (http://www.colan.org) and capitalised on further opportunities that can be gained from open standard interfaces for process simulation.

The CAPE-OPEN (CO) Physical Property Data Banks (PPDB) specification defines a standard set of interfaces for connecting thermophysical property data banks with user programs, allowing the automatic exchange of property data and of model parameters.

Allowing process simulator users to choose from any CO compliant PPDB is a major milestone for Computer Aided Process Engineering (CAPE) users. Independent PPDB suppliers can now make their information available to CAPE users in a plug and play environment, and companies can use their proprietary PPDB in the same fashion. A process model result is only as good as the model itself and the data it uses, so having the PPDB CO standard is a critical step forward to the successful implementation of CO principles in the CAPE marketplace.

SIMO 2002 conference (Systems for Information, Modeling, & Optimization), Toulouse, France, October 2002. CD-Rom Proceedings from http://www.ensiacet.fr/PROGEP/

Processus de standardisation pour l'interopératbilité des composants logiciels de l'industrie des procédés

Jean-Pierre BELAUD — **Laboratoire de Génie Chimique CNRS, INPT - ENSIACET**
Bertrand BRAUNSCHWEIG — **Institut Français du Pétrole**
Lars VON WEDEL — **RTWH Aachen**
Kerry IRONS — **Dow Chemical**
Michael HALLORAN and Daniel PIÑOL — **Aspen Technology**

Abstract:

Open software architectures are the way forward for the next generation of CAPE (Computer Aided Process Engineering) tools. The CAPE-OPEN (CO) standard achieves true plug and play of process industry simulation software components. Traditional simulation environments are closed monolithic systems. The resulting bottlenecks in interoperability, reuse and innovation have led to the CAPE-OPEN and Global CAPE-OPEN projects. These projects represent a collaboration between the chemical and petroleum refining industries, academics, and software suppliers, all with the same goal of defining a standard for component-based approach to process simulation.

SIMO 2002 conference (Systems for Information, Modeling, & Optimization), Toulouse, France, October 2002. CD-Rom Proceedings from http://www.ensiacet.fr/PROGEP/
Full paper available on http://www.prosim.net/english.html?page=publication.html

Interoperability concept in a COM thermodynamic server architecture. Example of integration in Microsoft® Excel™.

Alain Vacher and Philippe Guittard, ProSim SA

Abstract:

This article presents the new StarDust® thermodynamic server architecture developed by ProSim. From their origin, simulation tools have had to respond to a more and more demanding market and to adapt to the new hardware and software technologies. Today, they have to satisfy, among others, criteria such as interoperability, integration and reusability. The StarDust® Research and Development project, centred around a new software architecture, aims to provide such an environment. Although founded on an owner specification, this project integrates CAPE-OPEN standard and rests on the Microsoft® COM/DCOM middleware, widely diffused within its Windows® operating system. Within StarDust® framework, great care was taken in the thermodynamic server development, rightly considered as the cornerstone of any simulation application in process engineering. These server concepts make it possible to take advantage of the new architecture capacities, which can be illustrated by an example of integration in Microsoft® Excel™.

SCGCh 2002 Canadian Chemical Engineering conference (Société Canadienne de Génie Chimique), Vancouver, Canada, October 2002 (http://www.csche2002.ca/home.html) and as a poster at CIQ 2002, Barcelona Spain, November 2002.
http://www.ub.es/congres/9mediterraneo/

Towards a Standardisation of Optimisation Software

Chouaib Benqlilou, Santiago Bel, Antonio Espuña and Luis Puigjaner - Universitat Politècnica de Catalunya, Chemical Engineering Department
Michel PONS, ATOFINA

Abstract:

Optimisation Solvers are required and put to use at different levels of plant operation and design from Process Synthesis to Data Reconciliation and others. While the increasing improvement of computer performance and the development of new, efficient, and robust optimisation algorithms, favour the usage trend observed, the adaptation of these solvers to such new scenarios remains expensive in time, cost and implementation effort. Furthermore, in general, the existing solvers are black box systems so their integration in any application may prove difficult.

An efficient solution to overcome these drawbacks is to standardise solver communication with client applications in a consistent, efficient and secure way by designing a well-defined interface that ensures interoperability and transparency. Along this line, the CAPE-OPEN MINLP interface specification (CAPE-OPEN standard 1.0) has been recently proposed and is now supported by the CAPE-OPEN Laboratories

Network (CO-LaN).

Universitat Politècnica de Catalunya (UPC) has developed a software prototype by wrapping different kinds of Solvers from simple Linear Programming (LP) to complex Mixed Integer Non-Linear Programming (MINLP). The solver selected to be wrapped is part of CPLEX from ILOG (ILOG CPLEX 2001) and the implementation uses COM technology. It shows that the CAPE-OPEN Interface Specification for MINLP solvers is operational and that it is possible to develop MINLP solvers that are CAPE-OPEN (CO) compliant.

Considered as an help to developers, a Tester for MINLP solvers has also been specified and developed by UPC under contract from the CO-LaN. This Tester, a part of the CO Tester suite already targeted at Unit Operations, Thermodynamic, Physical Properties Data Banks components, will be freely distributed and used to validate the consistency and compliance towards the CAPE-OPEN MINLP Interface Specification of the pieces of software that implement it.

Software Architectures and Tools for Computer Aided Process Engineering, Editors Bertrand BRAUNSCHWEIG and Rafiqul GANI. Elsevier Science, B.V., ISBN: 0-444-50827-9, 2002 http://www.elsevier.nl

Software Architectures and Tools for Computer Aided Process Engineering

Peter Banks, BP International Ltd.
Jean-Pierre Belaud, Laboratoire de Génie Chimique CNRS INPT-ENSIACET
Kerry IRONS, The Dow Chemical Company
Tom Malik, ICI
Wolfgang Marquardt, Jörg KÖLLER, Alexander KUCKELBERG, and Lars von Wedel, RWTH Aachen
Michel PONS, ATOFINA
Luis Puigjaner, Universitat Politècnica de Catalunya
Sergi Sama, AspenTech
Bryn Stenhouse, BP International Ltd.
Tom Teague, Protesoft
Malcolm Woodman, BP International Ltd.

Abstract:

Computer Aided Engineering (CAPE) implies the use of computers and/or computer aided methods and tools in the solution of process and product engineering problems. CAPE software, as for many other classes of software, is becoming increasingly powerful, increasingly complex, increasingly better, increasingly used, and, last but not the least, increasingly diverse. The range of applications of CAPE tools is overwhelming: from physical property database searches to complex plant-wide dynamic optimisation problems solved in real time.

2003

FOCAPO 2003 conference (Foundations of Computer Aided Process Operations), Coral Springs, Florida, USA, January 2003. http://www.cheme.cmu.edu/focapo/

Missions of the CAPE-OPEN Laboratories Network

Jean-Pierre Belaud, Laboratoire de Génie Chimique CNRS INPT-ENSIACET
Michel PONS, ATOFINA
Kerry IRONS and Werner Merk, The Dow Chemical Company
Peter Banks, BP International Ltd.

Abstract:

The CAPE-OPEN Laboratories Network (CO-LaN) is the internationally recognised user-driven organisation for the testing and management of the CAPE-OPEN standard targeted at Computer Aided Process Engineering (CAPE) tools. The standard defines rules and interfaces that allow applications or components to inter-operate. The CO-LaN Society also helps to facilitate implementation of standard interfaces in commercial solutions such as AspenPlus™ from Aspen Technology Inc., Hysys.Process™ from Hyprotech, gPROMS™ from PSE Ltd., VALI III from BELSIM SA, INDISS from RSI, etc ... The CO-LaN Society acts as a new player in the process modelling area and proposes a different business model.

Any Feedback ?

Please submit comments and feedback to Kerry.Irons@colan.org . Only the authors are responsible for statements or opinions contained in articles.

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