

- General Information
- Download
- Standard Specification
- CO-LaN Catalog
- CO Support
- Request for Bids
- News
- Newsletter
- CO Update Issues
 - > CO_Update_articles
 - > CO Update 6
 - > CO_Update_7
 - > CO_Update_8
 - Latest News
 - Processium Member Profile
 - CO Update Survey Results
 - EPA Pollution Prevention Tool
 - INPT CO Course
 - Interoperability Lessons Learnt
 - SolidSim Simulator Project
 - New Thermo Standard v1.1
 - > CO_Update_9
 - > CO_Update_10
- Links
- Home

CAPE-OPEN UPDATE, Volume 8

CAPE-OPEN UPDATE is a publication of the CAPE-OPEN Laboratories Network (CO-LaN), a non-profit consortium for the development of the CAPE-OPEN standard.

STAFF LISTING:

Kerry Irons, Editor

Editorial Board: Peter Banks, Bertrand Braunschweig, Celeste Colantonio, Ronald-Alexander Klein, Werner Merk, Hans Pinggen, Michel Pons

Technical Support: ADDUCE GmbH

CONTENTS

- *Editorial - CO-LaN Consultancy On Offer*
- *Introducing Werner Merk, CO-LaN's New President*

Latest News

- *Hans-Horst Mayer Receives the 2003 CAPE-OPEN Award*
- *VMGSim by Virtual Materials Group, Inc.*
- *US EPA Seeks Post-Doctoral Research Candidates*
- *CO-LaN Members meeting in Leipzig, 12-13 February*
- *What's Up on the CO-LaN Web Site*

Member Profiles

- *Processium*

Technical Articles

- *US EPA's Metal Finishing Facility Pollution Prevention Tool (MFFP2T), by William Barrett, Paul Harten, EPA*
- *SolidSim Solids Processing Simulator, by Joachim Werther et al., TUHH*
- *"Lessons Learnt" from the Interoperability SIG*
- *INPT CAPE-OPEN College Course Review, by Jean-Pierre Belaud*
- *The Updated Thermo and Physical Properties CO Standard, by Richard Szczepanski*

CO Update Survey Results : Feedback on Your Feedback

User tips and current issues

EDITORIAL - CO-LaN Consultancy On Offer

The CAPE-OPEN Laboratories Network has undertaken a new initiative to aid the CAPE-OPEN community in its efforts to develop and implement CO compliant applications. The CO-LaN Board of Directors proposed, and the CO-LaN members have approved a mechanism to provide support for applications development with the following objectives:

- To catalyze the production of CO components by removing the difficulties of achieving CO-compatibility
- To secure the services of key CO experts in the vendor organizations
- To provide an added incentive for companies to join CO-LaN as full members

A portion of the CO-LaN budget will be used to contract appropriate service providers to assist third party developers of CO components to ensure that CO-compliance was achieved. Each CO-LaN industrial member is able to nominate one project per year, and the developer can have up to 2 days of assistance, paid for by the CO-LaN, for the implementation of the CO standards. So far, four consultants have been approved:

- AspenTech, www.aspentech.com , for all aspects of the use of CAPE-OPEN Unit, Thermo and Common interfaces in COM software components (contact: Sergi Sama, sergi.sama@aspentech.com)
- RSI, www.rsi-france.com for the use of CAPE-OPEN Unit and Thermo interfaces in both steady-state and dynamic CAPE-OPEN-compliant software components, particularly for real time COM applications. (contact: Didier Paen, Didier.paen@rsi-france.com)
- Universita Politecnica de Catalunya , www.upc.es/eq for the use of all CAPE-OPEN major interfaces in CAPE-OPEN-compliant software components, in both CORBA and COM applications. UPC provides access to small teams of students to assist in project development. (contact: Prof. Luis Puigjaner, lpc@eq.upc.es)
- Dr. Jean-Pierre Belaud, for the use of CAPE-OPEN Unit, Solver and SMST interfaces in CAPE-OPEN-compliant software components, particularly in CORBA project applications. Advice on all CAPE-OPEN interfaces and documentation. ENSI provides access to students for assisting in project development. (contact: Jean-Pierre Belaud, JeanPierre.Belaud@ensiacet.fr)

This service is yet another example of how the CO-LaN is taking concrete steps to facilitate the development and implementation of CO compliant components, not to mention the offer of a significant benefit for CO-LaN members. Details available through the [CO Support](#) tag.

Kerry Irons, Editor

CO-LaN Elects New President

At the recent CO-LaN members meeting in Leipzig, Germany, Werner Merk was elected as the new President. A little background:

Werner Merk is the Global Process Technology Consultant in Dow's Global Process Engineering department. In this role, Werner is responsible to define the vision and implementation plans for the core competencies in Global Process Engineering to provide improved technology solutions to Dow's Businesses. Werner is also accountable for commercialization of new technology in large capital projects in his areas of expertise.

Werner has a broad background in process and engineering technologies and is responsible for developing and maintaining internal and external networks with peers and colleagues, and has a leading role in Dow's Process Modelling efforts.

Werner holds a Ph.D. in Chemical Engineering from the University (TH) of Karlsruhe, Germany. After spending 4 years with Unilver, he joined Dow in 1984 in the Stade Bisphenol/Epoxy Plant. He has gained further experience from assignments in Manufacturing and Engineering, in process technologies such as MDI, propylene oxide, and polycarbonate, and core technologies such as Solids Processing and Process Modeling.

USER TIPS

Remember to visit the CO-LaN web site, then click [Standard Specification](#), to better understand both the method and the opportunity of implementing CO standards. If you are a CAPE software developer, you will find CO testers and the CO standards documentation. If you are a CAPE software user, you will find guidance on the use of CAPE tools in a CO-compliant environment. There is a great deal of information on the web site to guide you and offer insight.

Feel free to contact a CO-LaN member to help you focus your activities. These people can answer questions, discuss the philosophy of CO standards, direct you to CO standards experts, and give you a glimpse of current and future activities.

CURRENT ISSUES

The CO-LaN Special Interest Groups (SIGs), are up and running to refine existing standards, expand them as needed, and define new standards. The current SIGs, SIG leaders, and current focus areas are:

- INTEROPERABILITY - Peter Banks, BP (peter.banks@which.net). Interoperability Support for testing software interoperability.
 - THERMODYNAMICS - Jens Schmidt, Dow (jsschmidt@dow.com). For implementation, maintenance, and management of existing interfaces. Expansion into polymers and solids.
 - UNIT OPERATIONS - Celeste Colantonio, Shell Chemical (celeste.colantonio@shell.com). For implementation, maintenance, and management of existing interfaces. Expansion into dynamics.
-

BACK ISSUES OF CAPE-OPEN UPDATE

You can view back issues of CAPE-OPEN UPDATE on the CO-LaN web site - please go to News, then CO Update Issues

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COMING EVENTS, CO-LaN PRESS RELEASES AND OTHER CURRENT NEWS

Visit the CO-LaN website, then click [News](#) for the latest information!

CO tours are designed to show an organisation's technical professionals and technical leaders how to implement CO standards for their CAPE. Feel free to request one for your organisation.

Wizards are now developed for Unit Operations and Thermodynamics and are available through AspenTech/Hyprotech and through the CO-LaN web site.

The CO COSE (CAPE-OPEN Simulation Executive) tester is now ready and available on the CO-LaN web site.

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CAPE-OPEN Update Subscription

If you want to «subscribe» or «unsubscribe» CAPE-OPEN Update, please send an email to technologyofficer@colan.org with subscribe or unsubscribe as subject, respectively. If you need to contact the CO-LaN about the distribution list (if you have trouble unsubscribing or have questions about the list itself), please contact webmaster@colan.org

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- [General Information](#)
- [Download](#)
- [Standard Specification](#)
- [CO-LaN Catalog](#)
- [CO Support](#)
- [Request for Bids](#)
- [News](#)
 - [Newslist](#)
 - [CO Update Issues](#)
 - > [CO_Update_articles](#)
 - > [CO Update 6](#)
 - > [CO Update 7](#)
 - [CO Update 8](#)
 - > [Latest News](#)
 - [Processium Member Profile](#)
 - [CO Update Survey Results](#)
 - [EPA Pollution Prevention Tool](#)
 - [INPT CO Course](#)
 - [Interoperability Lessons](#)
 - [SolidSim Simulator Project](#)
 - [New Thermo Standard v1.1](#)
- [Links](#)
- [Home](#)

LATEST NEWS

- ***Hans-Horst Mayer Receives the 2003 CAPE-OPEN Award***
- ***VMGSim by Virtual Materials Group, Inc.***
- ***US EPA Seeks Post-Doctoral Research Candidates***
- ***CO-LaN Members meeting in Leipzig***
- ***What's Up on the CO-LaN Web Site***

CAPE-OPEN 2003 Award

The CAPE-OPEN Laboratories Network presented the third CAPE-OPEN Award to Hans-Horst Mayer from BASF in recognition of his outstanding contribution to open process simulation. The award was made on February, 13th, 2003 by Peter Banks, secretary of the CAPE-OPEN Laboratories Network (CO-LaN), during the CO-LaN members' meeting in Leipzig, Germany. The official Annual General Meeting, hosted by Dow, was attended by around 20 members from around the world.

In his presentation speech, Mr Banks said:

"I first met Hans-Horst in 1994 in Snowmass, Colorado at a FOCAPD meeting – a very nice place to meet someone incidentally. We had been thinking in BP for some time about the value of having a plug and play standard for process simulation and FOCAPD seemed like a good place to discuss it. Unfortunately, it didn't raise much interest at that time, but, as it turned out, it did raise just enough. Hans-Horst stood up and strongly supported it. We had a brief discussion and then we all left.

Life went on and BP got support from the EU project PRIMA to submit a plug and play proposal to the EU

Framework IV. We then discovered that the German IK-CAPE consortium was proposing to submit a very similar proposal and that this was as a result of Hans-Horst's persuasion and persistence. Both proposals were merged and after much struggle eventually became CAPE-OPEN, which finally started in 1977.

Of course that wasn't the end of Hans-Horst's involvement. Once CAPE-OPEN was under way, he continued to play a central role by running the team developing the Thermodynamics standard and participating in the management of the project. By the time he retired at the end of the CAPE-OPEN project, he was firmly established as one of its founding fathers. It's quite likely that without Hans-Horst's quiet determination in the early stages, CAPE-OPEN would not have happened at all."

Congratulations, Hans-Horst!

VMGSim Released by Virtual Materials Group, Inc. www.virtualmaterials.com

Virtual Materials Inc., Calgary, Alberta is pleased to announce the release of VMGSim, a cost effective and powerful steady state process simulation software package to predict the detailed behaviour of process units and manufacturing plants. VMGSim will accurately model and predict the behaviour of most process units in Oil and Gas, Refining, Petrochemical and Chemical industries.

- VMGSim features a fully integrated graphical I/O system powered by Microsoft Visio™
- Process schematics can be created using the integrated Visio™ graphics engine
- Excel™ spreadsheets can be seamlessly imbedded as unit operations in your flowsheet model
- The comprehensive and accurate property package engine is powered by the COM compliant component, VMGThermo.

VMGSim is a fully interactive and non-sequential modular simulator. It is designed to take advantage of two

characteristics related to the way process modelling problems are solved. VMGSim propagates as much information as possible through the flowsheet as soon as you enter the information, forwards and backwards from the entry point. VMGSim continuously monitors the information available in the flowsheet and as soon as degrees of freedom are satisfied, flash calculations are invoked, information is calculated and again propagated as described above. This design enables robust solutions to highly integrated processes and allows the modeller to start a model from the most convenient place without worrying about specific calculation sequences.

US EPA Seeks Post-Doc Researchers

The United States Environmental Protection Agency's National Risk Management Laboratory (NRMRL) is recruiting for Post-Doctoral candidates from a broad range of disciplinary backgrounds. While this is a general job posting, chemical engineers awarded these positions may have an opportunity to work on process simulation projects involving development of CO compliant software components. For the full text of the 2004 Post-Doctoral announcement, a brief description of the areas of research, and how to apply, please go to: <http://www.epa.gov/ORD/NRMRL/postdocfy04.htm>

The posting closes April 30, 2004.

CO-LaN Leipzig Meeting

CAPE-OPEN Laboratories Network held its Annual General Meeting, 13th February, 2004

Full members present:

BASF
BP
Dow

Ronald-Alexander Klein
Peter Banks
Werner Merk

| | |
|-----------------|------------------------------------|
| IFP | Bertrand Braunschweig |
| Shell Chemicals | Celeste Colantonio and Hans Pingen |
| Total | Michel Pons |

Associate Members present:

| | | |
|---------------|------------------------------|---------|
| AspenTech | Sergi | |
| Sama | | Fantoft |
| David Cameron | | |
| HTRI | Joseph Holmes | |
| NEL | Alan Scott | |
| PSE | Costas Pantelides | |
| SimSci | Neil Forster and Thomas Koup | |
| TUHH | Matthias Pogodda | |
| UPC | Luis Puigjaner | |

Individual Members present:

Hans-Horst Mayer

Membership : CO-LaN has 6 full members and 26 associate members. This represents a loss of 1 full member and a gain of 4 associate members. The issue of increasing the number of full (industrial) members remains a high priority for the management board, but all members were also asked to spread the word to their contacts.

Management Board : The board members in 2003 were:

| | | |
|-----------------|-----------------|-----------|
| IFP | B. Braunschweig | President |
| Dow | W. Merk | Vice- |
| President | | |
| Total | M. Pons | Treasurer |
| BP | P. Banks | Secretary |
| Shell Chemicals | H. Pingen | Member |
| Dow | K. Irons | Member |
| Shell Chemicals | C. Colantonio | Member |

Status Report - Bertrand Braunschweig . The board had monthly phone conferences or physical meetings, which dealt with decisions about Request for Bids and contracts, the 5 missions of CO-LaN and votes for new members. The contracts for Thermo 1.1 plug and tester have been successfully completed. Also contracts for

specification polishing and component catalogue production have been completed and web site maintenance and development is in place.

SIGs : There were 3 active SIGs, which are reported on below.

Web site . The CO-LaN web site is now managed by Adduce, using the OpenCMS content management system. It has a new “Component Catalogue” section and contains the CO Update newsletter in HTML form.

Marketing & Dissemination . The existing CO-LaN brochure has been retained and the CO Award scheme is continuing. During the year, presentations were made at FOCAPO, ICheaP6, AICHEMA, ECCE4 and ESCAPE-13 and a paper was submitted to Petroleum Technology Quarterly. Other publicity was obtained from the AspenTech/Fluent press release and via the AspenTech web site section on open standards. Three issues of CO Update were released.

Training . The world’s first “CO-compliant” university course was held at ENSIACET, Toulouse . Fourteen students successfully completed the course and developed a CO-compliant unit operation component. Further information is in the specific presentation on this subject on the CO-LaN web site.

Financial Report - Michel Pons . The overall level of expenditure in 2003 was € 72,273.14, whereas the fees collected were € 60,000. However, because of a one-off funds transfer from the EU for tester development under the Global CAPE-OPEN project, a surplus of € 37 ,147.21 was generated, which means that the total funds available at the end of the year were € 121,850.94. Some comments on the budget line items for 2004:

- **User Priorities** . This is expenditure on the Consultancy Services activity, which is explained below.
- **Dissemination** - This expenditure covers the fee for hosting the web site and allows for attendance at 4 conferences.
- **Standard Maintenance** - This allows for 10 days work on polishing standards documentation.
-

Testing - The tester suite needs to be kept up-to-date, particularly in the areas of PPDB, UNIT and MINLP. Also an allowance has been made for the possible acquisition of a computer for interoperability testing.

- **Training Facilitation** - No allowance has been made for 2004.
- **Administration** - This covers taxes, bank charges and limited support for Management Board meetings.

CO-LaN Consultancy Services - Peter Banks & Sergi

Sama . The objectives of this new service are: to catalyze the production of CO components by removing the difficulties of achieving CO-compatibility; to retain the services of key CO experts in the vendor organizations and to provide an added incentive for companies to join as full members. This will be done by allocating a proportion of the CO budget to contracting service providers to provide consultancy on CO-compliance to component developers approved by the Management Board (see Financial Report above). Each full member will be able to nominate one component per year to receive this service, with the remaining consultancy budget being allocated by the Management Board. A Request for Bids has been launched and 5 bids received. So far, 4 have been approved and shortly the first contract, with AspenTech, is expected to be signed.

SIG Reports

Thermodynamics ([Werner Merk](#), now to [Jens Schmidt](#)) -

After restating the charter and key responsibilities for the SIG and listing the current 11 members, the report went on to state the key events in 2003. These were: implementation of v1.0 in Aspen Plus 12.1 and resolution of speed issues; publication of downloadable report on optimization tricks for speed issues; production of IDL and Type Library for v1.0 implementations; functional specification for v1.1 finalized; extensions for solids agreed; SolidSim committed to implement v1.1 and TUHH joined CO-LaN and Thermo SIG. Goals for 2004 include: support for implementation of v1.0 and assistance with speed issues; support for implementation of v1.1 in SolidSim; verification of solids extensions of v1.1 and identification of next areas of interest.

Michel Pons then reported on the production of prototypes of the v1.1 specification, which extends and generalizes v1.0. These prototypes were produced by UPC (Tester) and Infochem (Property Package and Property Calculator). As a result of experience with the prototypes, some clarification has been made to the v1.1 document and some minor general issues raised. Overall, there were no fundamental problems in implementation, which was relatively straightforward and efficient.

Unit ([Celeste Colantonio](#)) - The main priority for 2003 was to extend the Unit specification to handle modular dynamic simulation. New unit categories and methods have been defined and specified and the IDL, component diagram and documentation extended. A pilot implementation was made in the RSI package INDISS, which worked smoothly and gave the same results as the equivalent simulation using all native INDISS units. Maintenance of the existing Unit specification was ongoing and took account of the relevant “lessons learnt” by the Interoperability SIG below. Goals for 2004 include: implementation of extended standard in D-SPICE and gPROMS; interoperability testing of dynamic components; further extension of the standard to include more types of basic component; external review of extended standard and ongoing maintenance of existing standard.

Interoperability ([Peter Banks](#)) - Main achievements in 2003 include: demonstrating successful use of unit parameters in Aspen Plus and HYSYS, which shows that the standard is capable of handling this behavior satisfactorily and that commercial CO implementations now allow activities such as optimisation and custom reporting; gPROMS thermo socket shown to be compatible with the latest version of the standard; gPROMS application gO:CAPE-OPEN produces interoperable CO-compliant unit components. In addition, 20 “lessons learnt” were gleaned from CO implementation experiences collated by the SIG. Goals for 2004 remain broadly similar, with emphasis on providing tools to assist in implementation and testing of CO components and limited direct testing when PRO II facilities become available.

Members Presentations and Demonstrations

gO:CAPE-OPEN ([Costas Pantelides](#)) - This presentation showed how gO:CAPE-OPEN fits into the gPROMS family of products from PSE and explained its function. It provides the ability for process engineers to include advanced gPROMS models in CO-compliant steady-state flow sheeting packages in a fully consistent manner, without the need for gPROMS programming. The model can be created separately by gPROMS specialists and packaged by gO:CAPE-OPEN so that it appears as a normal unit in the flow sheeting package. This behavior was demonstrated using a high-fidelity, rate-based reactive absorption model, built in gPROMS, running in an Aspen Plus simulation of a CO₂ removal process. This work was done using the standard CO Unit interface, which proved to be satisfactory for the purpose without modification.

SolidSim ([Matthius Pogodda](#)) - This presentation described the SolidSim Project, which is funded by AiF and involves 11 universities and an industrial advisory committee. It builds on work previously funded by VW-Stiftung. The aim is to develop a flowsheet simulator for solids processes. These processes are poorly served by existing simulators, because of the complexity of the description needed for the materials and processes involved. The presentation described the structure of the simulator and its use of CAPE-OPEN interfaces. Because the existing CO interfaces are developed for liquid/gas materials, extensions to the standard have been proposed by TUHH. The presentation finished with a demonstration of a simulation of a cascade of hydrocyclones separating fines from sewage sludge.

Elections of Management Board for 2004

All of the current Management Board stood for re-election and were duly re-elected, although with some changes in function and the addition of new members:

| | | |
|-----------------|-----------------|-----------|
| Dow | W. Merk | President |
| Total | M. Pons | Treasurer |
| BP | P. Banks | Secretary |
| IFP | B. Braunschweig | Member |
| Shell Chemicals | H. Pingen | Member |
| Shell Chemicals | C. Colantonio | Member |
| BASF | R.-A. Klein | Member |

Dow

K. Irons

Member

B Braunschweig stood down as President, although he remains on the Board. The meeting expressed its appreciation for his long and outstanding service at the head of CAPE-OPEN, Global CAPE-OPEN and CO-LaN. W Merk was elected in his place and C Colantonio and R.-A. Klein joined the Board as members.

Visit the Updated CO-LaN Web Site

With a new server and new features, there's a lot on offer at the updated CO-LaN web site (<http://www.colan.org>):

- From the [General Information](#) tab you can access our extensive FAQ list, see demos, get a membership application, and download a handy copy of the CO-LaN brochure that you can use to explain the CO-LaN to others in your organisation.
- From [Download](#) you have access to migration support, the CO tester, and help with COM-CORBA bridging.
- The [Standard Specification](#) tab gets you all the versions of the standard (v0.9, v0.9.3, v1.0, and v1.1). It's the heart of what you need to implement CO compliance.
- Clicking on the [CO-LaN Catalog](#) tab gives you access to a wide array of products and projects from the CO-LaN members (and others). It makes very interesting reading!
- The [CO Support](#) tab gives you access to CO-LaN approved consultants who can help you with migration and implementation projects. See the information on this new service in the editorial in this edition of CO Update
- Click on [Request for Bids](#) if you're interested in bidding on projects hosted by the CO-LaN.
- The [News](#) tab takes you to a chronological current events list as well (of course!) to current and back issues of the CO Update. Typical of the current list is information on the next CO-LaN members meeting, new standards and software tools on line, press releases on new software and implementations, calls for bids, new members, and so on. Keep up to date and keep in touch.
- Our [Links](#) area takes you to all kinds of interesting web sites

relevant to CAPE.

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- [General Information](#)
 - [Download](#)
 - [Standard Specification](#)
 - [CO-LaN Catalog](#)
 - [CO Support](#)
 - [Request for Bids](#)
 - [News](#)
 - [Newslist](#)
 - [CO Update Issues](#)
 - > [CO_Update_articles](#)
 - > [CO Update 6](#)
 - > [CO_Update_7](#)
 - > [CO Update 8](#)
 - [Latest News](#)
 - > [Processium Member Profile](#)
 - [CO Update Survey Results](#)
 - [EPA Pollution Prevention Tool](#)
 - [INPT CO Course](#)
 - [Interoperability Lessons](#)
 - [SolidSim Simulator Project](#)
 - [New Thermo Standard v1.1](#)
- [Links](#)
- [Home](#)

CO-LaN Member Profile

Processium is a company providing service in process conception, simulation, sizing and optimisation. Its main fields are thermodynamic, process modelling, and separation technologies.

Processium

- designs and scales-up industrial processes for oil refining, chemical and pharmaceutical industries
- bridges the gap between chemical synthesis and basic engineering
- is committed to help its customers from initial stages to plant production in close relationship with other project partners (engineering companies, manufacturers)
- finds the best technology for each separation problem

Processium's customers are European companies for chemistry, pharmacy and oil refining (Rhodia, Aventis, Speichim-Processing,...).

Processium CAPE activities:

Processium has two main fields of activity :

- Process Engineering conception
- Development of process conception software tools.

As a process engineering conception company, Processium is a wide user of CAPE tools (physical-properties data banks, simulation tools, Process Synthesis tools...).

As a CAPE-tool developer, Processium is currently developing a software tool for modelling liquid-vapour equilibria. This tool will provide thermodynamic data and model parameters

adjustment. This tool has to be able to communicate with the other CAPE software tools.

Contact Processium, UCBL 1 - Bâtiment Raulin - 43
Boulevard du 11 Novembre 1918 - 69622 Villeurbanne Cédex
– France <http://www.processium.com> , Phone: (+33)
4.72.44.84.32 Fax : (+33) 4.72. 43.13.30 -
processium@processium.com

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- [General Information](#)
- [Download](#)
- [Standard Specification](#)
- [CO-LaN Catalog](#)
- [CO Support](#)
- [Request for Bids](#)
- [News](#)
 - [Newslist](#)
 - [CO Update Issues](#)
 - > [CO_Update_articles](#)
 - > [CO Update 6](#)
 - > [CO Update 7](#)
 - [CO Update 8](#)
 - [Latest News](#)
 - [Processium Member Profile](#)
 - > [CO Update Survey Results](#)
 - [EPA Pollution Prevention Tool](#)
 - [INPT CO Course](#)
 - [Interoperability Lessons](#)
 - [SolidSim Simulator Project](#)
 - [New Thermo Standard v1.1](#)
- [Links](#)
- [Home](#)

CO Update Survey Results

In the second half of 2003, we undertook a survey of CO Update readers to better understand your interests and to improve the newsletter. The survey was short - just 6 questions - and the answers were scored on a 5 point scale, with 5 being the most favorable, 3 as neutral, and 1 being least favorable. Here are the questions, and the average of the **responses**:

I find the CO Update newsletter useful: 4.0

I wish to continue to receive CO Update: 4.6

My organization is capturing value through the use of the CO standards: 3.1

I would like more technical content in the newsletter: 3.7

I would like more editorial content in the newsletter: 3.0

I would like more current events information in the newsletter: 3.5

Overall, the respondents were quite positive about the value of the newsletter and wished to continue to receive it. Generally, the CO community wants more technical information and to be kept up to date on meetings, conferences, seminars and other current events. I promise to keep my editorials short!

Not surprisingly, at the time of the survey (3Q03) most organizations were not to the point of getting significant value from the CO standards. The recent updates of

AspenPlus, gPROMS, Hysis, and ProSim Pro/II were all just hitting the marketplace at that time, and the number of CO compliant "3rd party" software components was just starting to grow. The value of the CO standard is growing continuously through the efforts of the readers of this newsletter.

Of course no survey would be complete without the ability to offer **comments**, and below are representative of the feedback we received:

- There is a lot of potential to capture value for a specialty chemical company but this means more widespread adoption of the standards as well as interfacing between different types of packages to process modelling packages, e.g. supply chain modelling, fluids modelling, control system modelling, finite element modelling, data modelling and statistical packages as well as standard mathematical tools such as Statistica, MATLAB, Mathcad, etc. Ideally COLAN could take these on as specific objectives, with time-scales and a wider community of academics, tool vendors and process companies.
- If possible, we'd like more about success stories, and new functionalities (from the user point of view) which are only possible by using CO.
- Not using CO is temporary state, I still hope.
- We provide water industry simulators; CO is not yet needed, but I wish to keep abreast of what is happening.
- Analysis of new functionality and actual implementation case studies by companies would be very useful to us in deciding if / when we might want to get more involved.
- Information on how the CO and GCO standards are being used and what activities are in progress is useful.
- We need more in-depth information on how the

standard is actually used in industry, what the experiences are and what needs for further developments have been identified. Further, there should be a regular update on the route the suppliers are taking. Both ideas are quite difficult to implement, I am afraid, but these are the issues I am hearing quite frequently.

- I am glad to be a reader of your news and sharing information with my colleagues.
- A more complete newsletter would be maybe more useful.
- I enjoy receiving updates!
- Keep the good work up.
- I would like a printable copy - I hate looking at the thing on screen and it is more difficult to circulate within the office.

Organizations responding : ICI, SimSci, AspenTech, Shell, Fantoft, Norsk Hydro, WRc Group, Bayer, RSI, BP, Solvay, Shell. TU Delft, Degussa, Polish Fertilizer Research Institute, IFE, Univ. Wisc., Sulzer, Fluor, Degussa, Cardiac AS, UOP, University of Salerno, RWTH, Lund University, Roche, University of Brazil Rio Grande, Rhodia, ProSim, Infineum, Air Products, Dow, ENI Technology, University Magdeburg, French National Agricultural Research Institute - INRA, Intec - Argentine Technical University, Ecole Polytechnique de Montréal, InfoChem, Linde LE.

Thanks to all who took the time to reply to the survey!

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CO-LaN

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[Home](#)

- General Information
- Download
- Standard Specification
- CO-LaN Catalog
- CO Support
- Request for Bids
- News
 - Newslist
 - CO Update Issues
 - > CO_Update_articles
 - > CO Update 6
 - > CO Update 7
 - CO Update 8
 - Latest News
 - Processium Member Profile
 - CO Update Survey Results
 - >EPA Pollution Prevention Tool
 - INPT CO Course
 - Interoperability Lessons
 - SolidSim Simulator Project
 - New Thermo Standard v1.1
- Links
- Home

The US EPA's Metal Finishing Facility Pollution Prevention Tool (MFFP2T)

William Barrett, Ph.D., P.E

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United States Environmental Protection Agency

The United States Environmental Protection Agency has developed a pre-release version of a process simulation tool, the Metal Finishing Facility Pollution Prevention Tool (MFFP2T), for the metal finishing industry. This article will details the features the current version of this tool. We also provide a brief overview of additional components that can be added to the tool in order to aid metal finishing facilities in evaluating pollution prevention options, identifying and managing the facility's supply chain, aid the facility in documenting regulatory compliance, and support creation of an environmental management system.

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The United States Environmental Protection Agency is currently developing a pollution prevention tool for use in the metal finishing industry, which will be built around a process simulation program. Currently the tool has the ability to create and edit a flowsheet, a database of chemical species that may be present in the simulations, a database of chemical reactions, and basic unit operations of interest in the metal finishing industry. This paper will present the current status of the process simulation software, and provides some information regarding future work to be conducted as part of developing the tool.

User Interface

The primary aspect of any computer program that user must encounter is the user interface. In an effort to develop an interface that is intuitive for the user, and obtain feedback during the development process, this section will present an overview of the current user interface. Upon opening the program, the user will be presented with a blank flowsheet upon which the process flow diagram for the simulation can be constructed. The user is presented with two toolbars; the first contains standard Windows functionality (*e.g.*, loading and saving files, printing the document, etc.) and the second provides for the insertion of unit operations and flow streams. By clicking on the desired unit operation, the user can build the flowsheet.

A flowsheet is constructed by first selecting the source object, which represents the "storage tank" where chemical feedstocks are kept. The source tanks are the only place where a solutions' chemical composition can be set directly; that is, concentrations in other tanks are calculated from models, such as material balances, equilibrium models, plating models, or other appropriate process models. As unit operations are added to the flowsheet, flow streams are used to indicate the material flow from one unit operation to the next. Because unit operations may have multiple connection points, each expecting a particular type of stream, once the user identifies the source and destination unit operations, the program brings up a port selection dialog box that asks the user to select the appropriate source and destination ports. The user then selects the correct ports and the flowsheeting software makes the appropriate connections.

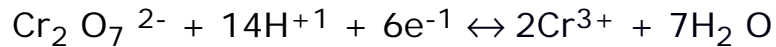
As indicated above, the composition of the material in the feedstock is set using the material editing form. This form currently consists of two parts; the first part allows the user to set the concentrations, temperature, pressure, and flow rate of the material stream. The second part is used to add compounds in the property package to the current material object. When a compound is added to the feed stream, its concentration is automatically set to 0. It should be noted that the calculations are all conducted in System International (SI) units, such as molarity (moles/liter). A future modification of the code will be made to allow users to set concentrations in more familiar units, such as milligrams per liter (mg/L), or other traditional units.

The program utilizes two databases; first a chemical database and the second is a reactions database. The chemical database, or property package, is a listing of all chemical species available for use in the program. Currently, a limited test property package has been built, which will be expanded for the release versions. The property package can be accessed and edited using a Property Package Edit Form. This form presents the name, formula, molecular weight, Gibbs Free Energy, and other appropriate information and physical properties of the chemical compound.

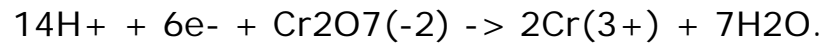
The reactions database actually consists of four separate databases, as follows:

- acid/base reactions
- solution reactions
- coordination/complexation reactions
- and Oxidations/Reductions reactions

Creation of separate databases was selected because it separated the different chemical concepts associated with each of the four distinct types of chemical reactions that commonly occur in water chemistry. Further, the user needs only to consider one type of reaction at a time. The reaction editor also consists of two windows; the first is the list of reactions, and the second lists the chemical species in the reaction. A reaction is created by selected and adding the chemical species involved in the reaction. Once the species have been added, the stoichiometric coefficients are added. The stoichiometric coefficient of a reaction product is positive and the coefficient of a reactant is negative. For example, the coefficients of the oxidation reduction reaction:



are -1 for the dichromate ion ($\text{Cr}_2\text{O}_7^{2-}$), -14 for the hydrogen ion (H^{+1}), -6 for the electron (e^{-1}); 2 for Chromium(III) (Cr^{3+}), and 7 for water (H_2O). The standard electrode potential is also added for use in calculations. The resulting reaction will appear in the reaction database as:



The reactions to be used for a particular unit operation or material flow can be selected using a reaction selection dialog box. Each type of reaction can be selected using the appropriate tab in the selector. Once all desired reactions have been selected, the reaction set is used to construct a tableau as described in Morel and Hering (1993).

Once the flowsheet has been constructed, it can then be calculated by selecting the calculate command from the calculate menu item. The calculate command goes through each unit operation and requests that it calculates itself.

Status of Process Simulator

The EPA has completed the basic simulation package, and is now working to create a model of a Nickel Plating line. The simulation package is based on the CAPE Open standards and EPA will likely make it available as an open source package. At this time, the EPA can distribute the Visual C++ source code and will provide information as needed to individuals interested in creating software to work within the simulation package. The simulation package provides base classes that can be inherited to create unit operation and stream object models. Further, users can create objects for use in the simulation package in either Visual Basic or C#.

Future Work

The process simulator has been created based on the CAPE-OPEN standards developed for chemical process simulation software (CAPE-OPEN Project Team 2000). As previously stated (Barrett and Harten 2003), the intention of using the

CAPE-OPEN standards is to utilize process simulation tools developed for the general chemical process industry in the metal finishing pollution prevention tool. Currently, the USEPA has updated the (W)aste (R)eduction algorithm (WAR) (Young and Cabezas 1999) so that it can interact with a CAPE-OPEN compliant material object and calculate the WAR value for the process stream.

Having the ability to utilize process simulators to evaluate pollution prevention options will provide industry with a powerful tool for waste reduction. The simulator will allow process engineers to estimate the reduction in the quantity of waste generated by a process change without having to take the process offline and modify the process. Additionally, multiple process options can be tested and the results compared in a relatively short period of time, giving the engineer the ability to select the best combination of process modifications.

Future improvements can include the ability to combine the process simulation with a cost analysis program to provide the facility with the ability to conduct an engineering economic analysis of the process modification. In this way, the facility can be proactive in identifying waste reduction opportunities that can reduce waste disposal costs and increase operational efficiency. This would enable the engineer to determine which pollution prevention options are cost effective and communicate the potential cost reductions to management.

Through the ability of the simulator to communicate with other computer programs using either the CAPE-OPEN interfaces, or interfaces developed by others, such as the OLE for Process Control (OPC) interfaces (OPC Foundation, undated), the effect of process conditions on product quality can be evaluated. The process simulation tool and process control packages can then be combined with other applications such as statistical quality control tools, enabling the process engineer to evaluate the effect of process changes on the quality of the finished product. Improvements in product quality will result in less product rework, reducing the mass and/or toxicity of waste production.

Creation of an environmental management system (EMS) enables the facility to evaluate the environmental footprint of the facility. Properly implemented EMSs have the potential to improve corporate image, achieve financial savings through

improved efficiency, lead to competitive advantage, and achieve measurable reductions in pollution. Using process simulation tools as part of EMS development can streamline the evaluation of the environmental lifecycle of the process. As EMSs are often initiated or used as part of an environmental compliance program, the process simulation tool, combined with the process control package, can be used to assist in record-keeping functions necessary for regulatory submissions.

Summary

The USEPA has an ongoing effort to create a pollution prevention tool for use by the metal finishing industry. This tool is being constructed around a process simulator. The process simulator will be capable of calculating the quantity of wastes generated by a particular process flowsheet. Once the amount of wastes generated can be estimated, various options for waste reduction can be investigated and analyzed.

The current status of the project is a basic simulation tool where users can enter unit operations and concentrations of chemical present, and calculate the equilibrium concentrations of the chemicals present. As the tool is developed, additional unit operations will be added to enable the simulation of a metal plating line.

Future work includes the evaluation of the environmental impacts associated with the chemicals present in the generated wastes, as well as methods that can be employed by facilities to reduce the quantity of, or hazards associated with the generated wastes.

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- Newslist
- CO Update Issues
 - >CO_Update_articles
 - >CO Update 6
 - >CO Update 7
 - >CO Update 8
 - CO Update Survey Results
 - EPA Pollution Prevention
 - Tool
- >INPT CO Course
 - Interoperability Lessons
 - Latest News
 - Processium Member Profile
 - SolidSim Simulator Project
 - New Thermo Standard v1.1
- Links
- Home

Information Technologies II:

An education program involving CAPE-OPEN standard

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Keywords

Education, Information technologies, Component and object-oriented approach, middleware, open architecture and interface, unit operation, dynamic simulation, operator training systems, CAPE-OPEN, INDISS tool

Abstract

This short paper introduces an education program that was done in the ENSIACET School of INPT University. The program mixes academic and industrial contributions. The main objective is to teach information technologies, especially open architecture and component based approach, and then to apply these concepts to process engineering using an industrial tool and an open standard. This standard, CAPE-OPEN, is taught. It allows the students to integrate their compliant unit operations in the INDISS environment provided by RSI company.

Contents

- Context
- Overview of Information Technologies courses
- Objectives
- Planning and content
- Students' evaluation
- Scenario of workshop 4
- Main results, reactions and perspectives

Context and overview of Information Technologies courses

ENSIACET (www.ensiacet.fr) is a "grande école" enclosing 5 departments that trains high level scientists and engineers in the field of the transformation of matter from the molecular scale to industrial process scale. Please refer to the appendix for more information on ENSIACET.

The education program called **Information Technologies II** (IT II) is organized for the third-year students who have selected the **Process Engineering and Computing** department. This program comes after a course called **Information Technologies I** (IT I) done during the second year. This document is not really a technical paper. It is a description of IT II education project involving CAPE-OPEN and our feedback on this pioneering experience.

The first general course IT I is mainly focused on (web) technologies. It discusses the Internet, computing history, information systems, needs for integration and interoperability, open computing, standardization process and web dynamic/semantic. We introduce HTML, Microsoft ASP, XML and Java principles (object-oriented concepts and C++ programming language are taught in other courses). We demonstrate the merging of Web and object/component technologies. The practical classes of IT I are essentially focused on HTML development.

Then **Information Technologies II** intends to study more advanced technologies and to work with industrial applications. In IT I, students learn the basics and are exposed to the CO standard, working with the RSI application. IT II moves to specialisation with more depth on the CO standard and an industrial example of process engineering (in this case from Total). This program gathered **two education units** (2*9h30) and **two conferences** (2*1h20) at end of 2003. 14 students followed the units and 32 students attended to both conferences.

- The education units are done with contribution of **Laurent Testard** and **Philippe Thiabaud** from **RSI**. Laurent Testard is computing sciences expert and is in charge of RSI product development. Especially he develops the technical classes. Philippe Thiabaud is process engineering expert and leads project on Operating Training Systems. He builds dedicated simulators starting from generic classes provided by INDISS environment. Altogether they bring their expertises on computing sciences and process engineering aspects in the scope of INDISS solution.
- The conferences are proposed by **Michel Pons** from TOTAL and **Didier Paen** from RSI. Michel Pons speaks also for the *CO-LaN organization*. Didier Paen manages the research and development of the INDISS product.

Objectives

The main objectives of this program are **to teach information technologies and to apply them in the scope of process simulation thanks to CAPE-OPEN standard (CO)**. We identify several topics in our initial objectives:

- **IT:** software architecture, open standards, middleware and interface concept, component based approach, software engineering, UML modeling, design-implementation with "round-trip engineering" (code generation), C++ component development, perspectives (web services)
- **Process engineering:** INDISS solution, motivations and usage of dynamic simulation, dynamic simulation principles in sequential modular, dynamic unit operation, development of a made-to-order dynamic simulator, demonstration of a complex industrial Operator Training System with DCS emulation.
- **IT & Process engineering:** CAPE-OPEN standard principles, CO-LaN organization, CO components demonstrations, CO compliant unit operation development, integration of third-party application in compliant environment.
- **Others:** CAPE software provider, industrial feedback from a large and small company, industrial software development project, standardization process and community common effort, connection with INPT research for the CO initiative.

In addition, the students practice the following tools in the Windows 2000 environment, having already used Visual C++ and Rose previously.

- *Borland VisiBroker for C++ 4.0*, an ORB for CORBA middleware
- *Microsoft Visual C++ 6.0*, an integrated development environment
- *Rational Rose Enterprise 2002*, a UML modelling tool
- *INDISS 1.5*, process modelling and simulation environment
- *CAPE-OPEN 1.0* and *dynamic unit operation interface*, a standard for the interoperability and the integration of process engineering software components

The INDISS environment (INDustrial and Integrated Simulation Software, www.rsi-france.com) provides a simulation framework for the whole process life cycle. INDISS integrates up-to-date technologies and avoids the duplication of modelling and simulating efforts by creating a single model for all the different purposes of modelling and simulation. It specifically covers five kinds of needs: Operability and Controllability Studies, Operator Training Simulation (OTS), Process Operation Support, Advanced Process Control and Process Optimisation. The students practice OTS functionality through two specific flowsheets, *Depropaniser* and *Drum*.

Planning and content

The students have followed seven theoretical classes, seven practical classes and both conferences. Theoretical class elements include: Introduction, Internet, Software architecture, Paradigms, Middleware technologies, Conclusion & Perspectives, Dynamic simulation and INDISS tool while practical classes propose four workshops. The TOTAL and CO-LaN conference deals with TOTAL activities, CO, CO-LaN and CO interoperability videos while the RSI talk presents RSI software solutions, software engineering, development methodology and the RSI CO strategy. The planning is summarized in the following:

| Course no. | Type | View | Educator(s) |
|------------|------------------|---------------------|-------------------|
| 1 | Theoretical | Web solutions | Belaud |
| 2 | Theoretical | Web solutions | Belaud |
| 3 | Theoretical | Web solutions | Belaud |
| 4 | Theoretical | Web solutions | Belaud |
| 5 | Theoretical | Web solutions | Belaud |
| 6 | Theoretical | Web solutions | Belaud |
| 7 | Workshop 1 | Web solutions | Belaud |
| 8 | Workshop 2 | Web solutions | Belaud |
| 9 | Workshop 2 | Web solutions | Belaud |
| 10 | Theoretical | Process engineering | Thiabaud, Testard |
| 11 | Workshop 3 | Process engineering | Thiabaud, Belaud |
| 12 | Workshop 3 | Process engineering | Thiabaud, Belaud |
| 13 | Workshop 4 | Process solutions | Testard, Belaud |
| 14 | Workshop 4 | Process solutions | Testard, Belaud |
| 15 | TOTAL conference | Process solutions | Pons, Belaud |
| 16 | RSI conference | Process solutions | Paen, Belaud |

The students work on three kinds of problems with a web solutions development view, a process engineering view and a process software solutions integrator view. Each view is practiced in the workshops.

The aim of *workshop 1 and 2* is to apply the web solutions development view. The keywords are object-oriented concepts, C++, UML, CORBA components, interface and unified process. The application consists of developing two basic software components which are based on CORBA middleware technology. A component offers a service on the network acting as the *business model server*. The second component plays the role of *presentation client*. These

two components are compliant with an interface. This interface is previously designed jointly following a process based on UML modelling. 8 diagrams are drawn during the different phases of the process. This process is defined by the *analysis, design, specification, implementation* and *validation/deployment* phases. Some readers can remember the process followed in CO projects. The CORBA IDL is not difficult. It is just analyzed since it is generated automatically from the interface or component diagram with the Rose tool. We design a basic interface on the basis of a bank account and the interface is "standardized" at the level of the classroom for interworking of components issued from each group. Once both components are developed, they are deployed on the INPT-ENSIACET network. The component clients identify, contact and call the component servers on the same and remote hosts. During workshops 1 and 2, the students operate Rose, VisiBroker and Visual C++.

Workshop 3 proposes a usual process engineering view. At this level, our students' new knowledge resides in the *dynamic simulation in sequential modular* and in the use of INDISS CAPE tool, knowing that our students are trained in simulation with the ProSimPlus product from ProSim SA (www.prosim.net). The students have to use the tool, understand its graphical interface, and use and run simulations on the *Depropaniser* flowsheet. They run different scenarios, such as changing the reflux controller on a distillation column, and then they analyze the simulation results.

The *workshop 4* mixes process engineering and IT according to the process software solutions integrator view, knowing that the introduction of the CAPE-OPEN standard has been discussed and worked with previously. The students develop their own compliant unit operation making use of an INDISS template and then they plug the resulting component into the CO compliant INDISS environment flowsheet. The template, a set of C++ files, provides a basis for the technical layer such as the CO Parameters, constructors, destructors, etc. The *NetworkCompute()* method is empty and has to be completed once the template is understood. The flowsheet is a basic Drum. We did not use the depropaniser flowsheet from workshop 3 due to technical reasons. The underlying middleware technology is COM and the programming language is always C++.

Students' Evaluation

Before starting the workshop 3 and 4, the students had to produce two one-page reports on the CAPE-OPEN initiative and on the INDISS tool. In addition to web resources, a scientific paper on CAPE-OPEN and the introduction to INDISS document are provided (from J.P. Belaud and B. Braunschweig, CAPE-OPEN: interopérabilité de composants logiciels pour la modélisation de procédés physico-chimiques, ICSSEA 2003, Software & Systems Engineering and their applications). The objective of this first work was to prepare the courses from 10 to 16 that unify academic and industrial contributions.

After the completion of IT II program, each group of students had to make a report on the workshops. This year the evaluation was essentially on workshop 1, 2 and 3. The UML model, the associated materials that document the development process, and the thinking on a set of questions and comments were the core of the report. Also the description and the analysis of a scenario of workshop 3 were requested. No formal evaluation was done on workshop 4 for the first presentation of this program.

Scenario of workshop 4

The main practical objective of workshop 4 is the development of a CO compliant dynamic unit operation (UO) component and its integration within a CO compliant environment. The actual scenario was shared in three parts such as:

First step: objectives and recording of COM components

- To open a Windows session (development account with specific rights)
- To get CO dynamic UO Visual Studio workspace

To record CO components and to identify CO categories in registry

Second step: template for CO compliant dynamic UO development

- To understand the Visual Studio workspace for development of CO UO
- To see the software design with UML modelling
- To analyze the C++ source files: CCOArcExampleImpl.h/.cpp, ...
- To build the project and to get the arc component («empty » UO, no process engineering model)
- To customize the arc rgs file: Name, Categories, ...

Third step: development of arc component and integration in INDISS

- To add a CO Parameter (Cv)
- To implement the process engineering model (flow calculation)
- To build the arc component (.dll file)
- To deploy the arc component on an RSI laptop available on the education network
- To integrate it within the INDISS environment
- To run the drum flowsheet and to check the arc component dynamic behaviour (see Figure 3)

One technical problem was identified the day before workshop 4. The final integration on ENSIACET Windows machines was not possible. This is due to a complex problem related to the COM component record of arc component in the Windows registry. To do it with an administrator account did not solve the problem. Therefore, once the components were built by students on ENSIACET machines, the deployment, integration and validation were realized on RSI laptop.

Main results, reactions and perspectives

The education program called Information Technologies II was successfully completed at the end of 2003 at INP Toulouse-ENSIACET University. An associate professor and industrial contributors from RSI and TOTAL were involved. To announce and develop such a program is not so obvious for many reasons; pedagogic difficulties, industrial availability, agendas, financial costs, INDISS installation, classroom Windows configuration, licensing, etc. Working with the CO dynamic unit operation specification coupling with an in-development INDISS version for the workshop 4 has especially intensified the challenge. So we have to say that we are very satisfied by the outcomes of this first offering of the course.

As a result the effective education benefits are:

- ***Concepts and methodologies:*** software architecture, standards, development process, standardization process, component based approach, middleware technologies, IDL interfaces, design-implementation connection, automatic code generation, UML modelling, process engineering oriented integration, services oriented perspectives, dynamic simulation, OTS, R&D industrial project.
- ***Technologies:*** CORBA, VisiBroker, INDISS, Rose, C++, CAPE-OPEN standard, CAPE-

OPEN compliant COM components.

We got a fervent reaction from ENSIACET education staff. The education chief thanks the industrial representatives for their contributions, for their support for limiting education program costs and asks for ongoing support for this project the next year. From the perspective of students, a feedback form reveals that they are clearly satisfied. In summary, 2 students said us "correct", 8 "good" and 4 "very good".

Of course, many ways of improvement can be considered such as to extend the schedule of workshop 4, to work with a more "complex" UO model, to have the same INDISS process flowsheet for workshop 3 and 4 and to integrate and run CO components on ENSIACET PCs. Also it would be interesting to have an industrial conference on the scope of IT & process simulation in the 2nd year.

In a long term view, an interesting way would be to *re-use the unit operation model* the students have developed in the *process modelling and simulation course* during their second year. More connections with other education courses would expand the innovative IT II program.

Acknowledgments

The students, the education chief and I would like to thank Laurent Testard, Philippe Thiabaud, Michel Pons and Didier Paen for their contributions to this inventive project and their active and enthusiastic involvement. INPT-ENSIACET thanks RSI for the availability for the workshops of INDISS product with no charge and CO-LaN for covering Michel Pons' travel costs. Personally I just want to add I really enjoy developing this program with them.

About the Author

Jean-Pierre Belaud led research and development efforts in the areas of Computer Aided Process Engineering. Mainly since January 1997 he participated to the exciting project of a standardisation process. So he was involved in the projects that resulted in the CAPE-OPEN standard and the associated CO-LaN consortium. He was in charge of these projects for the INPT institute. Qualified in chemical and computing engineering in 1996, he brought his expertise in the CAPE and software development fields. Since September 2003 he is associate professor at INPT-ENSIACET University (www.ensiacet.fr). He is especially in charge of IT and computing education programs for Process Engineering and Computing department and Industrial System Engineering department. On the research side, he is working in the Process Systems Engineering team of CNRS-LGC ([see website](#)).

More information on ENSIACET and Process Engineering and Computing department

ENSIACET (A7, www.ensiacet.fr) is a "Grande Ecole", which is strongly committed to training engineers of a high scientific and technical standard, in the field of transforming material, from its molecular form to large scale industrial processes. A7 is one of three engineering schools) of INPT (Institut National Polytechnique de Toulouse, www.inp-toulouse.fr).

As all French "Grandes Ecoles", ENSIACET recruits students via a national competitive examination, taken at the end of a two-year common core curriculum, called "Superior Mathematics" and "Special Mathematics" following Baccalauréat, equivalent to A-level. The students are awarded their Engineer Degree after the completion of three years at ENSIACET; this degree is equivalent to a Master of Science degree.

A7 has guaranteed for a long time two main objectives: training and research, which are carried out in tight collaboration with the industrial sector. Four research laboratories are connected to A7:

LGC, Chemical Engineering

- LCA, Agro-Industrial Chemistry
- LCCFP, Catalysis, fine chemistry and polymers
- CIRIMAT, Material Science and Engineering

Today, A7 welcomes 750 students, who benefit from a high level scientific and technical environment, 105 teachers and researchers, and also from the support of a technical and administrative staff of about 100 people. Created in 2001 by the merging of the ex Chemistry (ENSCT) and Chemical Engineering (ENSIGC) Schools, A7 inherits of one century of Education and Research experience, with more than 4000 awarded engineers.

The A7 Process Engineering and Computing engineer has a deep theoretical and practical background in Chemical Engineering, the mastery of mathematical, numerical and computing methods and tools and a general training in economical, human and social sciences.

The A7 Process Engineering and Computing engineer is able to manage the process all along its life cycle. By using modelling, simulation and optimization techniques, he has a rigorous and integrated approach to process synthesis, design and operation, taking into account economic constraints, but also safety, environmental, flexibility and controllability constraints. This training gives an engineer the skills to efficiently contribute to multidisciplinary projects in the chemical, petrochemical, nuclear, bio and food industries.

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- Download
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- CO Update Issues
 - >CO_Update_articles
 - >CO Update 6
 - >CO_Update_7
 - CO_Update_B
 - Latest News
 - Processium Member Profile
 - CO Update Survey Results
 - EPA Pollution Prevention Tool
 - INPT CO Course
 - >Interoperability Lessons Learnt
 - SolidSim Simulator Project
 - New Thermo Standard v1.1
- Links
- Home

Interoperability SIG Lessons Learnt

The Interoperability Special Interest Group has the goal of making sure that CO compliant Process Modelling Environments (PMEs) and Process Modelling Components (PMCs) will interoperate as required. The SIG's 2003 summary report contains a section called 'Lessons Learnt' which includes a number of recommendations to developers of PMEs, PMCs, and Property Packages as well as guidance to the CO-LaN Thermo and Unit SIGs for future standard changes. This information is somewhat detailed, but it provides useful insight for those affected, and may even be interesting reading for some users as well.

A full copy of the Interoperability SIG annual report is available from CO-LaN webmaster (see contact at page bottom).

The lessons to emerge from the tests and developments are catalogued below. Note that "CO standard" refers to an individual standard within the CO framework, e.g. the Unit Operation standard or the Thermo standard.

- All PMEs need to be able to trap CO components that use versions of the CO standards that are not supported by the PME.
 - **Attention: PME vendors**
- There is a need for a generic "interface reporting" component that will sit between the PME and PMC and report the information being passed between the two. This will greatly aid the debugging of CO interface implementations.
 - **Action: Interoperability SIG**
- Components and environments must be written **strictly** to the relevant standard.
 - **Attention: All developers**
- Specific examples of non-adherence found so far that need to be considered are:
 - CO Unit Operations must respect the basis qualifier in calls to getProp and setProp for a material object. Furthermore, the basis qualifier must be strictly enforced in PMEs
 - The type of value returned for a parameter must match the parameter's specification.
 - All string comparisons in CO components and environments must be case insensitive
 - A CO Unit Operation must not attempt to validate the material objects associated with its ports until it is asked to calculate. There is no guarantee that the material objects are valid until the calculation is requested
 - CO components must expect the correct return types when calling Material Object methods. For example, the specified return type for a call to GetComponentConstant of CapeArrayVariant is defined as VARIANT (i.e. any type) in the CO IDL. The use of CapeArrayVariant means that the variant returned will itself contain an array of variants – even if only a single value is being returned. The type of each variant in the array may be different depending on what data was requested.
 - **Attention: All developers**
- The CO testers should be able to diagnose all cases where code does not strictly adhere to the standard. We need to check to see if the testers need further development.
 - **Action: Interoperability SIG**
- For complete interoperability, all PMEs should implement a supported standard in full (but see discussion below). For example, a PME implementing the Unit standard should support Array variables, otherwise some CO Unit Operations will not work fully.
 - **Attention: PME Vendor s**
- However, this could be less onerous for vendors and clearer for purchasers, if the

standards were split into a number of logical sections. This would allow vendors to specify which sections of a standard their software supports, if they were unable to support it all. An example of this would be to move the CO Equilibrium Server into a separate section within the Thermo standard, so that a PME vendor can explicitly and easily state whether their PME does or does not support this feature. We request that SIGs with responsibility for standards should review and comment on this proposal.

- **Attention: SIGs with responsibility for standards**
- Component and Environment developers must take extra care to ensure that their code is bug free, since detecting bugs becomes more difficult with inter-operation of components from different suppliers. An example of this is a component which contains a memory over-write, which may only appear when the component is used in a particular way in a single PME.
 - **Attention: All developers**
- A new work-flow for the use of a CO Property System has been identified, as follows:
 - Open PME
 - Invoke CO Property System from within PME and open specific GUI for Property System
 - Load existing Property Package or create a new one
 - Close GUI for Property System and return to PME
 - Either select the required Property Package or have it automatically selected based on the choices made in the GUI for the Property System
- This work-flow is not currently supported by the CO Thermo standard, which expects that the required Property Package has been created before the user opens the PME. We suggest that support for this alternative work flow should be considered in a future version of the Thermo standard.
 - **Attention: Thermo SIG**
- A CO Property Package cannot currently assume that any calls it does not implement can be forwarded back to the material object it has been given, as the action to be taken in this situation is not specified in the standard. It is therefore possible that a material object will simply forward all calls relating to property calculations back to the Property Package associated with it. If the client is a Property Package this will result in recursive calls that will end in a crash.
 - **Attention: Property Package developers**
- It would however be useful if a CO Property Package could obtain the necessary pure component properties from the PME, rather than the component having to include its own pure component property databank. We suggest that a protocol for such a call-back should be considered for a future version of the Thermo standard.
 - **Attention: Thermo SIG**
- Furthermore, Property Packages that implement a sub-set of models (e.g. liquid density only) are not currently explicitly supported in the standard, although it may work in some PMEs. We suggest that this should be considered as a future enhancement to the Thermo standard.
 - **Attention: Thermo SIG**
- If a CO Property Package does not implement all the properties expected by a PME, then the PME needs to report this in a meaningful way. Note that the CO Thermo standard does not specify which properties should be made available by a Property System, but simply provides a full list of those that are supported by the standard. However, we suggest that there should be any easy way of identifying the properties available in any specific implementation of a CO Property System, either via the System itself or the PME it is being used in.
 - **Attention: PME Vendors and / or Property Package developers**
- A CO Property package may predict the existence of more valid phases than are supported by the PME in which it is being used. In this case the CO interface performs exactly as expected, but there is an obvious incompatibility between the component and environment and the effects are uncertain. The Thermo standard should be enhanced to at least document this scenario and provide suggested remedies, or the specification should be enhanced so that the interface itself can trap the problem
 - **Attention: Thermo SIG**
- The CO Unit standard does not support a "string" parameter; instead this needs to be implemented as an Option parameter. We suggest that string parameters should be added to the Unit standard. The specification for Option parameters needs to be clarified: is it

legal to have an Option Parameter with an empty Option list? Interoperability testing has shown that whereas one PME (HYSYS) allows this, another (Aspen Plus) doesn't.

- **Attention: Unit SIG**
- A CO Unit Operation must not change the current working directory of the application in which it is running. Any CO Unit Operation that displays a File Open dialog and allows a file to be selected from any directory will change the current working directory as a side effect. The correct mechanism is to save the current working directory before displaying the dialog and then to restore it afterwards.
 - **Attention: Unit Operation developers**
- The DLL for a CO Unit Operation must not be unloaded while the CO Unit is in use. Note that the provider of the CO Unit Operation can control the unloading of the DLL by implementing DLLCanUnloadNow.
 - **Attention: Unit Operation developers**
- CO Unit Operations should handle the failure of calls to optional or non-essential Material Object methods robustly.
 - **Attention: Unit Operation developers**
- CO Unit Operations must be correctly registered. In particular they must at least provide a value for CapeDescription\Version so that PMEs know which versions of the CO interfaces they support. In addition, PMEs should ignore Unit Operations (and other components) that do not have version specified.
 - **Attention: Unit Operation developers and PME vendors**

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[Home](#)

- General Information
- Download
- Standard Specification
- CO-LaN Catalog
- CO Support
- Request for Bids
- News
 - Newslist
- CO Update Issues
 - >CO_Update_articles
 - >CO Update 6
 - >CO Update 7
 - >CO Update 8
 - Latest News
 - Processium Member Profile
 - CO Update Survey Results
 - EPA Pollution Prevention Tool
 - INPT CO Course
 - Interoperability Lessons Learnt
 - >SolidSim Simulator Project
 - New Thermo Standard v1.1
- Links
- Home

Flowsheeting for Solids Processes

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While flow sheet simulation is a common method to design and optimize chemical processes involving only fluids, in solids processing it is still common practice to design one apparatus separately from the other. There is a lack of suitable methods to combine single apparatus models with a process model and to treat this process as a whole. The

present paper will elaborate the reasons for this situation and will present a concept and a program package under development, which will allow the application of methods of flow sheet simulation on complete processes, in which at least one major component is a solid.

Introduction

Today, flow sheeting program packages are commonly used in chemical engineering for the design of processes involving fluids. The simulation of processes which involve solids or solids and fluids is not as advanced, and it is common practice to design and optimize each apparatus separately from the others, neglecting its influence and dependence from the neighbouring processes. This allows finding optimal operating conditions for each unit operation or apparatus. But such a sequential optimization of individual units will not always lead to a global optimum for the whole process.

With respect to flow sheet simulation there are some major differences between fluid processes and solids processes, resulting from the dispersed nature of solids:

- While a fluid can be characterized by a limited number of concentrated parameters as temperature, pressure, composition and some compound specific parameters, a lot more information is required to describe solid particles, e.g. size, porosity, humidity, shape.
- Most of the additional parameters are distributed parameters, e.g. the particle size distribution. Even the composition of solid particles is often not homogeneous but has to be treated as a distributed parameter. And, of course a distributed composition of the solids will cause most parameters which depend on the composition of the solids to be distributed, too.
- In many cases a certain property may be dependent from another distributed property, e.g. during a drying process the water content of coarse particles will be higher than that of small particles, which dry

much faster than the coarse ones. But even particles of the same size will not have under any circumstances the same humidity: if there is a residence time distribution there will be a distribution of humidity within each particle size class. This leads to a hierarchy of dependent distributed properties.

- In many cases the exact composition of solids is not known (and often not of interest) as for example in the case of coal or sand. In these cases the solids have to be defined as their own species. This approach, however, makes it nearly impossible to obtain or calculate exact properties for this species without doing experiments.
- Even when the properties of single particles are known, generally applicable methods to calculate the bulk properties from the properties of the individual particles are often missing.
- The performance of an apparatus is often significantly influenced by the geometry and can not always be scaled easily; e.g. the diameter of a hydrocyclone is decisive for the separation process, influencing both the cut size and the separation sharpness.

The above mentioned differences require a numerical treatment of solids which strongly differs from the treatment of fluid components. Thus it is hardly possible to extend existing simulation packages for fluid processes to the simulation of solids processes without restructuring and re-implementing it from scratch. Distributed parameters require additional mathematical treatment, e.g. the fulfillment of population balances, which add new families of equations to the complex mathematics of flow sheeting systems and thus need new or adapted solvers.

For these reasons it was decided at the Hamburg University of Technology to put efforts into the development of a completely new system for the simulation of solids processes. These efforts led to a project together with 10 of the leading academic groups in particle technology from different German universities with the aim to develop a simulation system for solids processes called SolidSim. In addition, many industrial users of solids processes and suppliers for solids processing equipment contribute with

their expertise to this development. This two year project is now funded by the AiF (Arbeitsgemeinschaft industrieller Forschungsvereinigungen) within their ZUTECH program.

Objectives for the Development of SolidSim

The main objectives for the development of SolidSim as a flow sheet simulator for solids processes can be derived from the special requirements of solids processes as given above. Thus, the simulator should provide a stream structure, which allows a description of solids with distributed parameters, allowing also for a hierarchy of dependent properties. Furthermore mathematical methods and solvers must be provided which allow the treatment of population balances.

Even though the development is focused on solids processes, SolidSim should not be limited to them, but should allow also the simulation of related fluid processes. Since it is far beyond the scope of the present project to develop all model required for such a simulation by itself, an important requirement is to follow open standards which allow the inclusion of external modules into SolidSim or of SolidSim into other simulation environments. To achieve these aims it was decided to follow the CAPE-OPEN standards wherever possible and extend them in order to include the treatment of the distributed parameters for solids.

Another objective was to develop an open system such that new modules can easily be added, that different models for the same apparatus can be made available at the same time and that modules can easily be replaced by improved modules without affecting the whole system.

Besides these objectives concerning the inner functionality of the system there was furthermore the requirement to develop a user friendly system with an ergonomic easy-to-use graphical user interface (GUI), to allow engineers to build process following their view.

Modelling solids with distributed parameters and fluids significantly increases the heterogeneity of the mathematical equations to be solved. Since solving these equations requires quite different solvers, it was decided

not to use an equation oriented simulation approach but to build a block-oriented simulation system.

As software platform the Microsoft Windows[®] operating system family has been chosen.

Structure of SoldiSim

The program system was divided into three major parts: the simulation environment, the stream objects, and the model library with the unit models. The simulation environment provides the basis of the system. It provides the graphical user interface, some basic functionality as reporting, printing, saving and loading data, and it controls the calculation sequence. The material stream object provides the structures necessary to transport the information on the fluids and solids from one module to the next one, and to provide the modules with all properties of the materials needed by the modules. The Unit Model simulates a single apparatus or unit operation. These basic elements are connected by different interfaces as defined by the CAPE-OPEN-Standard. However, some interfaces had to be extended within this project for the treatment of solids parameters.

Additionally, communication with other simulation packages is also possible using the CAPE-OPEN interfaces. A detail flow sheet simulated with SolidSim may be used as one module in an external CAPE-OPEN compliant simulation environment, using standard interfaces for the communication. Another method is to incorporate modules from other packages as unit models inside the SolidSim environment or to use external property packages inside SolidSim.

Model Library

The model library is basically a collection of independent software modules containing one or several models for a certain apparatus or a unit operation. In the framework of the current project, a basic library with models for the most important solids process steps will be implemented. For each apparatus, models of different complexity and different requirements with respect to the input data will be used. This allows the use of different models in different

stages of the design process, e.g. quite simple models which need only a few, easy to measure or to estimate data in an early design phase and a more complex model with higher data quality requirements to simulate or optimize an existing plant.

The software modules are implemented as COM objects, so that they can be added and removed during runtime without influencing the remaining simulation system.

The modules communicate with the simulation environment using the CAPE-OPEN *ICapeUnit...* interfaces and with the connected streams for the handling of distributed parameters extended *ICapeThermo+...* interfaces. The *ICapeUnit...* interfaces are used to control the program logic and execution sequence, the *ICapeThermo+...* interfaces are used to query all information about the incoming materials. In the case of solids processes, additional information e.g. on the geometry of the apparatus is usually necessary; such information as well as model parameters have to be requested from the user by a user interface provided by each module. Usually only parameters purely related to the apparatus should be queried this way, but for some models, parameters related to the combination of apparatus geometry and solids properties are needed and also have to be queried this way.

In order to facilitate the development of a unit model, a 'base unit class' has been developed, which forms the basis of all currently developed modules. The task of this base unit is twofold, first it will hide all implementation details for the communication between the different software components from the "engineering oriented" developer of the unit model. The second task is to provide and ensure a minimal functionality, e.g. to copy input to output streams, to check mass balances, to provide methods for connecting streams to the ports of the apparatus, etc. In the simplest case the model implementer should only have to implement specific calculation and initialisation routines and to provide some basic information about entrance and exit ports.

Within the present project, the model library will be far from being completed, but for the most important areas of solids processing, models will be implemented. Below you can find a list of solids processing steps for which models will be developed together with the name of the responsible

project partner.

- Separation, classification, fluidisation, framework; Werther, Hamburg
- Simulation Environment; Gruhn, Hamburg
- Crystallisation, dissolving; Kind, Karlsruhe
- Agglomeration, granulation; Mörl, Magdeburg
- Crushing in mills; Peukert, Erlangen
- Filtration of fluids; Ripperger, Dresden
- Gas filtration; E. Schmidt, Wuppertal
- Separation processes in centrifuges; Stahl, Karlsruhe
- Convection drying; Tsotsas, Magdeburg
- Liquid sprayers; Walzel, Dortmund
- Dosing and conveying; Wirth, Erlangen

Stream Objects

One major development task in the project is the development of the stream objects, i.e. the structures which store the current status of a material stream connecting two subsequent models or units in the flowsheet and which have to provide the models with all properties of the incoming materials, i.e. fluids and solids. The material stream object mainly provides access to a compound list, a property package providing the thermo-physical properties of the compounds, a list of global constants and a phase manager.

While existing approaches could be used for the implementation of the fluid part and for the storage of concentrated properties, the implementation of the solids part with the distributed properties had to be newly developed.

The design goal was a structure which allows the efficient storage of and access to complex hierarchies of nested and dependent distributed solids properties. In addition, the stream object should be able to provide the information to the unit models in an appropriate manner, i.e. it should only give the information needed by the module, hiding all additional complexity.

The problem with the dependent distributed parameters will be clarified with the following example in which a gas cyclone is used to separate solids from a gas. The gas cyclone separates solids from a gas due to the centrifugal forces inside the vortex. Thus, the separation is governed by the terminal velocity of the particle in a centrifugal field. A further influence on the separation efficiency is the solids loading μ defined as solids mass flow divided by the gas mass flow. An increasing solids loading at the cyclone entrance increases the total separation efficiency and changes the fractional separation efficiency.

Now let us take a solids stream made up from two different kinds of solids with given particle size distributions and given densities. The simplest approach to calculate the separation efficiency would be to calculate the separation for the two compounds in sequence, but this not possible due to the interaction of the solids and due to the influence of the total solids loading at the entrance. The approach which is used here is to give the cyclone model the information in a manner as it is needed, i.e. to give the total gas flow, the total solids flow and a distribution of the terminal velocities of the solids, not distinguishing between the two different kinds of solids. Then the cyclone model gives back to the stream object the total solids separation efficiency and a movement matrix, i.e. the information about which mass fraction in each terminal velocity class is separated from the gas flow and which mass fraction could not be separated. The stream object then calculates from the movement matrix the separation for each particle size of each compound. Thus, the fact that the entrance flow was formed of different compounds is hidden from the cyclone model, which allows using a standard separation model, which is usually designed for only a single compound.

Similarly the separation of solids with a dependent distribution of humidity or any other property can be done

by the standard gas cyclone model, as long as the stream object is able to calculate the influence of the dependent property on the distribution of terminal velocities. Similar scenarios could be found for most of the solids processing steps.

In order to facilitate the calculations which have to be performed by the stream object, the properties for the solids are stored in an n-dimensional matrix with n being the total number of different properties under consideration. In this way the dependences between the properties are depicted without implying any hierarchy.

Status of the Simulation Package SolidSim

Currently all the basic structures as described above are implemented and first versions of the unit models have been implemented. Testing of the simulation system is ongoing using different processes we are kindly provided information on by industrial partners. One of the test cases simulated is a plant for the separation and dewatering of contaminated sewage sludge. The aim of this process is to maximize the amount of sand with low contamination and to minimize the amount of highly contaminated fines under the restriction that a certain allowed level of contamination of the sand is not exceeded. The flow sheet of this process includes several unit models, for example sieves, a hydrocyclone, decanter, elutriator and thickener.

For further testing we strive to simulate the multi stage evaporation of a caustic soda solution as occurring within the caustic soda process. Here the crystallization, including recycling of crystallization product, has to be calculated showing the ability of SolidSim not only to deal with pure solids processes but to be able to handle solid-fluid interactions as well.

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An Updated CAPE-OPEN Thermodynamics and Physical Properties Specification

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Introduction

The Thermodynamics and Physical Properties Specification (Thermo. spec.) was one of the earliest products of the CAPE-OPEN (CO) project. It was recognised that thermodynamic and physical properties were often at the core of a company's technology and that in-house physical properties were a major barrier to exploiting the full range of available simulation/modelling software. The CO project offered the possibility of taking the physical properties from one source and being able to use them across a range of applications through a standard interface. The original Thermo. Spec. was published in 1999 with a revision in 2002 [1]. Along with the Unit Spec., the Thermo. Spec. is perhaps the most used and useful of all the products of the CO project – so why do we need a new version?

The Thermo. 1.1 Spec. has grown out of an effort by the Global CAPE-OPEN Interoperability Task Force (ITF). The ITF had the task of demonstrating that the CO vision could work in practice by interchanging unit operations and physical properties between commercial process simulators. Although this effort has been successful it was by no means straightforward and many lessons were learned. Physical properties were at the root of many incompatibilities. It was obvious that the 1.0 Spec. required clarification but it also needed a fresh approach to move beyond the limited conception of 2-phase (vapour-liquid) equilibrium that informed its design.

This article describes the background and objectives of the Thermo. 1.1 Spec. and reviews some of the key features. The prototype implementations of the specification together with the draft document [2] are available on the CO-LaN website.

Objectives

The objectives we had in mind when formulating a new Thermo. spec. included the following:

- To improve the clarity - by removing ambiguities and defining the purpose and functionality of components in some detail. The target audience is implementers of physical property systems and their clients, the suppliers of process simulation software.
- To simplify implementation of Thermo. plugs and sockets by breaking down

functionality into simpler units and removing redundant features (e.g. the calcType specification).

- To improve reliability by defining exceptions for each method and by providing a complete range of methods to check the capabilities of a component.
- To support efficient implementations by simplifying methods and adding streamlined methods to handle the most frequently used calculations.
- To add new facilities and support future extensions. These include multiple phases, solids, completely general flash specifications, and distributed properties.

Software components

The Thermo. 1.1 Spec. describes four types of software components.

- Property Calculator (PC) – can calculate certain physical properties, possibly restricted to mixtures of particular compounds in particular phases.
- Equilibrium Calculator (EC) – can calculate the composition of mixtures, possibly restricted to mixtures of particular compounds existing in particular phases and subject to certain constraints.
- Property Package (PP) – combines the functions of a Property Calculator and an Equilibrium Calculator for a fixed set of compounds and phases. In the remainder of this article the Spec. will usually be discussed in the context of a PP.
- Property Package Manager – manages a set of Property Packages. It is responsible for instantiating Property Packages on request and may allow packages to be edited and/or created. This component has a very specific and simple function and will not be discussed further.

The purpose of these components is broadly similar to those defined in the 1.0 Spec. but we have (mostly) chosen different names to describe better their functionality and to emphasise the different interfaces and methods supported.

An additional component is the Material Object (MO) which provides access to the data describing a material (e.g. chemical species, composition...). The MO is used as a container to communicate between a Thermo component such as a Property Package and a client such as the Process Modelling Environment (PME).

Interfaces and Methods

In the 1.0 Spec. there is a one-to-one correspondence between software components and interfaces whereas in 1.1 there are more interfaces but each one may be implemented by several components.

The interfaces and their methods are summarised in the following list taken from a figure in reference [2]:

ICAPEThermo PropertyPackageManager

+GetPropertyPackageList()

+GetPropertyPackage()

ICAPEThermoPropertyRoutine

- +CheckSinglePhasePropSpec()**
- +GetSinglePhasePropList()**
- +CalcSinglePhaseProp()**
- +CheckTwoPhasePropSpec()**
- +GetTwoPhasePropList()**
- +CalcTwoPhaseProp()**
- +CalcAndGetFugacityCoefficient()**

ICAPEThermoEquilibriumRoutine

- +CheckEquilibriumSpec()**
- +CalcEquilibrium()**

ICAPEThermoUniversalConstants

- +GetUniversalConstant()**
- +GetUniversalConstantList()**

ICAPEThermoPhases

- +GetPhaseList()**
- +GetPhaseInfo()**
- +GetNumPhases()**

ICAPEThermoMaterial

- +GetPresentPhases()**
- +SetPresentPhases()**
- +GetSinglePhaseProp()**
- +SetSinglePhaseProp()**
- +GetTwoPhaseProp()**

+SetTwoPhaseProp()

+GetOverallProp()

+SetOverallProp()

+ClearAllProps()

+GetTPFraction()

+CreateMaterial()

+CopyFromMaterial()

ICAPEThermoContext

+SetMaterial()

ICAPEThermoCompounds

+GetCompoundList()

+GetCompoundConstant()

+GetConstPropList()

+GetNumCompounds()

+GetPDependentProperty()

+GetPDependentPropList()

+GetTDependentProperty()

+GetTDependentPropList()

ICapeThermoMaterial

This interface is implemented by a MO and it is used by any of the Thermo. components to communicate with a client. The methods are mostly concerned with getting and setting properties in the MO. For example, a PP might use `GetSinglePhaseProp` to get the temperature at which a calculation should be performed and `SetSinglePhaseProp` to return a calculated value.

ICapeThermoPhases

The methods of this interface provide information about the number and types of phases (gas, liquid, solid...) supported by a Thermo. component. It would typically be implemented by a PP, PC and EC component. More details about phases are given in a separate section below.

ICapeThermoCompounds

This interface is implemented by components that provide information about chemical species. The methods can be used to identify compounds and to request/provide property values for *pure* compounds.

ICapeThermoPropertyRoutine

The methods of this interface support property calculations. Properties may depend on a single phase, *e.g.* enthalpy, or they may involve two phases, *e.g.* K-values or surface tension.

ICapeThermoEquilibriumRoutine

This interface provides methods for carrying out phase equilibrium calculations where the overall mixture composition is fixed plus the values of two constraints such as temperature and pressure.

Uniform Structure

The methods giving access to properties and calculations have a uniform structure:

- Enquiry methods – return a list of the supported properties. *E.g.* GetSinglePhasePropList.
- Check methods – to allow a calculation specification to be checked prior to carrying out the calculation. *E.g.* CheckSinglePhasePropSpec.
- Calculate methods – to perform a calculation. *E.g.* CalcSinglePhaseProp.

This pattern is repeated wherever possible and appropriate.

Handling of Phases

The handling of phases in the 1.0 Spec. is rudimentary. An important advance in the 1.1 Spec. is the support of any number of phases and any types of phases. Information about the phases supported by a component is provided by the methods of the ICapeThermoPhases interface. A central concept is the phase label. This is an arbitrary string, *e.g.* "HydrocarbonLiquid," that is used to identify a particular phase and to refer to its attributes. The attributes provide information that helps client software or a human being understand what sort of phase the label refers to. A list of attributes is given in the following table.

| Phase attribute | Meaning |
|----------------------|--|
| state of aggregation | the physical state: vapor, liquid or solid |
| key compound | identifier of the compound that is expected to be present in highest concentration in the phase – this helps to distinguish multiple instances of, say, liquid phases. <i>E.g.</i> for an aqueous liquid phase the key compound would be water |
| excluded compound | this is the opposite of the key compound, <i>i.e.</i> identifier of the compound that is expected to be present in low or zero concentration in the phase |

| | |
|---------------------|--|
| density description | description that indicates the density range expected for the phase, <i>e.g.</i> Heavy or Light |
| user description | description to help the user or PME identify the phase |
| type of solid | description that provides more information about a solid phase, <i>e.g.</i> PureSolid, SolidSolution, Hydrate etc. |

A PP can support any number of phases, each with a unique phase label. The PME can use the ICapeThermoPhases interface to discover the number and types of phases supported. Although a PP may support many phases this does not imply that a client should make use of all of them. For example some PMEs may not be able to handle solid phases.

Phase Equilibrium Calculations

The methods of the ICapeThermoEquilibriumRoutine interface have been designed to make them as general as possible in order to allow for multiphase calculations and any type of flash specification. Within the scope of the 1.1 Spec. a phase equilibrium calculation must return the amounts and compositions of the phases at equilibrium (plus the temperature and pressure) given the overall composition of a mixture and the values of two constraints. There are no fixed identifiers for the type of flash but instead two specification variables are used to identify the constraints and the actual *values* of the constraints are retrieved using the MO. For example, in the simplest case of an isothermal, isobaric flash the constraints are the temperature and pressure themselves. This scheme allows for almost any flash specification.

A particularly important class of flash problems correspond to the specification of the temperature or pressure plus the amount (phase fraction) of a particular phase. This is a generalisation of the familiar P/T plus vapour fraction specification for vapour-liquid systems. Practical applications include the calculation of the water dew point or hydrocarbon dew point in oil/gas/water systems or the calculation of a solid wax formation temperature.

A PP may support a large number of phases but it is not necessary to consider all of the phases in any given equilibrium calculation. The SetPresentPhases method of the ICapeThermoMaterial interface may be used by the PME to define a subset of the phases supported by the PP that should be considered in a phase equilibrium calculation. For example, to allow for hydrate formation modelling in general a PP must support the following phases: gas, hydrocarbon liquid, aqueous liquid, solid ice, solid hydrate structure I, solid hydrate structure II. In a high temperature section of a process it may not be necessary to consider the solids so SetPresentPhases could be used to restrict the calculations to gas/hydrocarbon liquid/aqueous liquid. Of course the conditions may be such that an aqueous liquid phase does not form so SetPresentPhases would also be used by the Equilibrium Calculator in the PP to report the actual phases present at equilibrium.

Distributed Properties

It is recognised that some properties may not have a simple point value like the temperature or pressure. The Thermo. spec. already caters for properties that have an intrinsic vector or matrix structure like the fugacity or diffusion coefficient. A further possibility is a property that depends on a distribution that characterises a material. For example, the density of a particulate solid may depend on the particle size distribution. To allow for the possibility of properties with complex data structures the methods for setting and getting properties may return an interface pointer that can be used to invoke special methods to handle a property. A set of extensions for handling distributed properties has been proposed by workers at the University of Technology Hamburg-

Harburg to support the SolidSim project.

Efficiency Considerations

It is a common assumption that open interfaces present a penalty in terms of computational efficiency when compared with native interfaces. Work on the 1.0 Thermo. spec. showed that the penalty of using the CO interface could be reduced to a small margin but this required considerable care in programming both the PME Thermo. socket and the Property Package plug. The experience gained has been encapsulated in a document [3] which shows that a major barrier is overcoming the overheads of using COM. The lessons learned with the 1.0 Spec. have been incorporated in version 1.1 along with some important improvements to the interface structure and the methods.

ICapeThermoContext interface

When a PP is called with a request for a property calculation it needs to obtain information from the client using the MO. Instead of passing the MO reference as an argument to the calculation methods as was done in the 1.0 Spec. the 1.1 Spec. provides the ICapeThermoContext interface with a single SetMaterial method for this purpose. Any component that requires to access a MO must implement this interface. The change has some important consequences. The MO reference is set by the SetMaterial call and the PP can assume that the configuration of the MO remains unchanged until SetMaterial is called again. Thus any overhead associated with checking that the MO is valid or any initialisation of the PP that depends on the configuration of the MO (compound list, phase list) need only be carried out when SetMaterial is called instead of at every call for a property calculation or flash calculation. The new arrangement allows code to be simplified and, assuming that changes in configuration of the MO are not frequent compared with property evaluations, can make a significant improvement in calculation speed.

Calculation conditions

It is important to minimise the number of calls from one software component to another. Every property evaluation with the methods of the ICapeThermoPropertyRoutine interface requires that the temperature, pressure and composition of a phase be retrieved by the PP using the MO. The 1.1 Spec. optimises this operation by providing a special-purpose method GetTPfraction that fetches all the information in a single call rather than requiring three separate calls to the GetSinglePhaseProp method. Furthermore the arguments of all methods used to access properties are defined as input/output arguments even though their use is actually to provide output information. This means that efficiency savings can be made in setting up and reusing storage - the technical background is given in reference [3].

Fugacities

The most intensively used property is the fugacity coefficient [3] because it is the basis of all flash calculations. A special method is provided in the ICapeThermoPropertyRoutine interface to optimise this calculation. CalcAndGetFugacityCoefficient does just what its name suggests. The method is unusual in the CAPE-OPEN context because both calculation conditions (T, P, composition) and calculation results (fugacity coefficients and their derivatives) are passed as arguments. The MO is not used. This arrangement allows the overhead of procedure calls to be minimised.

Simplified Property Calculation Requests

The format of property calculation requests has been drastically simplified allowing for much improved software structure and consequent improvements in efficiency and maintainability. Two classes of properties are defined for mixtures. Single phase properties are those that depend on the state of a single phase, *e.g.* enthalpy, volume... Two phase properties depend on the state of two phases in equilibrium, *e.g.* K-values, surface tension... Separate methods are provided in the ICapeThermoPropertyRoutine interface to handle the two classes.

The structure of a method like CalcSinglePhaseProp in 1.1 is very simple – the arguments specify the list of (single-phase) properties and a *single* phase label. This should be compared with the equivalent 1.0 method CalcProp that allows a list of properties, a list of phases and a 'calcType' which indicates whether pure or mixture properties are required. The resulting multiplicity of possible property and phase combinations in CalcProp makes the organisation of the calculation procedure complex and difficult to optimise.

Exception Handling

The error handling strategy for CAPE-OPEN components is described in reference [4]. Although that document lists some exceptions for Thermo. 1.0 components there is no definition of the circumstances in which the exceptions might be raised.

The 1.1 Spec. includes a list of exceptions for each method of every interface and carefully describes the conditions corresponding to each exception. A great deal of time and debate was spent on this topic. The exception definitions were further refined as a result of the prototyping of 1.1 components (see below). Experience suggests that the present exception list should allow reliable and effective handling of error conditions for Thermo. components.

Prototyping

Prototype Thermo. 1.1 components have been developed by Infochem for the Co-LaN in conjunction with a parallel development of a new CO-Tester at the Universitat Politècnica de Catalunya. For more details of the CO-Tester see reference [5].

The components developed were a Property Package and a Property Calculator. Both are based on a very simple set of thermodynamic and transport property models for a limited number of compounds. The phases supported are vapour, liquid and aqueous liquid and two phase equilibrium calculations are provided: P,T flash and P,H flash. The Thermo. 1.1 interfaces are implemented in a Visual Basic wrapper that is completely separate from the calculation procedures which are contained in an independent dll. It is the intention of the Co-LaN that the prototypes should be available to help other developers that need to understand or implement the 1.1 Spec.

The prototyping exercise was a very useful experience. As a result the descriptions of the methods, arguments and exceptions were improved and clarified to remove ambiguities and to deal with unanticipated circumstances. In general the 1.1 Spec. was easy to implement and allowed for considerable simplifications compared with the equivalent 1.0 code which was used as a starting point.

Conclusions

The 1.1 Thermo. spec. is the result of a major collaborative effort between suppliers of process modelling software, users, physical property specialists and software specialists. It forms a basis for extending the current CAPE-OPEN standards to new areas of application including multiple phases, solid phases and distributed properties. Prototype implementations have demonstrated that the proposals are practical and useable.

References

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