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Editorial Notes

by Peter Rony and Karl Schnelle

# **CAST Communications - Spring 2005**

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In this issue, the editors are pleased to publish Ross Taylor's presentation at the CAST Awards dinner at the 2004 Annual Meeting. This address is in response to his winning the Computing in Chemical Engineering Award. Furthermore, the winners of the 2004 CAST Directors' Awards are announced in this issue. For the first time, we are also publishing the winning poster as well as the two Honorable Mentions.

In addition to all the CAST awards, please read the article by Michel Pons about the CAPE-OPEN Laboratories Network, a non-profit organization promoting standards for Computer-Aided Process Engineering (CAPE).

And don't miss the Quote of the Day by Albert Schweitzer.

#### Latest News

April fool, n. The March fool with another month added to his folly.

Ambrose Bierce, The Devil's Dictionary

**AIChE** 

Grid Computing

Now that SETI@home and others have popularized the technology, a new consortium has been organized by some big names: HP, IBM, Intel, and Sun. The non-profit Globus Consortium will give the auto, aerospace, and energy industries open source tools to develop grid computing systems. Issues still to overcome are reported to be a lack of business applications that accommodate the architecture of the grid and a lack of monitoring tools to track decentralized work on the grid. (Karen Epper Hoffman, Technology Review, 2 Mar 2005)

A Titan of Physics and the Conscience of Science "I always wanted to find out how the world is made, what it is made of, what holds it together, what makes it operate the way it does."

> Hans Bethe (1906-2005) See the Cornell Chronicle.

# Articles

**CAST Awards Dinner** 

by B. Wayne Bequette, CAST Division First Vice-Chair

We would like to congratulate again all the award winners announced at the 2004 CAST dinner: 2003 Directors' Award, 2004 W. David Smith Jr. Award, 2004 Outstanding Young Researcher, and 2004 Computing and Chemical Engineering Award. Details of these awards may be seen in Wayne's presentation [1070 KB, pdf] D. The original announcement occurred in the Fall 2004 newsletter.

Full presentation [1070 KB]



Wayne Bequette (I) presents Vince Grassi (r) with a plaque in appreciation for excellence and service as the 2004 CAST Chair.



... Sarette van den Heever (r) with the W. David Smith Jr. Award.







... Ross Taylor (r) with the Computing and Chemical Engineering Award.

Postcards [645 KB]



... Paul Barton (r) with the Outstanding Young Researcher Award.

#### Postcards from Austin, Computing in Chemical Engineering Award Address by Ross Taylor, Clarkson University

For his outstanding contributions to multi-component mass transfer and for developing the non-equilibrium approach to separation process modeling and design.

Ross' entire <u>address</u> [645 KB] to the attendees of the 2004 CAST Awards dinner may be downloaded in pdf format.

## 2004 CAST Directors' Award

by Richard D. Braatz, CAST Division Director

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On behalf of CAST, I am delighted to announce the winners of the eighth annual CAST Directors' Award for the 2004 AIChE Annual Meeting in Austin.

# Elizabeth Morel (speaker), Hui Zhao, C. Russell Middaugh, and Kyle V. Camarda, University of Kansas

"<u>Computer Aided Molecular Design of DNA</u>: Polymer Complexes using Solubility Correlations and Phase Diagrams" (paper 403k). The <u>poster</u> [315 KB, <sup>(k)</sup>] is available in pdf format.

The two students who did the work for the poster are Elizabeth Morel (on the left) and Hui Zhao (on the right).

Two Honorable Mentions were also given:

- "Excursion Potential in Cyclopentadiene Reactors in the Purification of Isoprene" (Paper 403af), Colin S. Howat\*, University of Kansas, Lawrence, KS. The poster [291 KB, <sup>()</sup>/<sub>2</sub>] is available from the university.
- "A Globally Optimal, Dynamic Based, <u>Operating Point Selection Scheme</u> for MPC" (Paper 414t), **Donald J. Chmielewski\*, Jui-Kun Peng**, Illinois Institute of Technology, Chicago, IL. The <u>poster</u> [343 KB, <sup>[]</sup>] is available in pdf format.

The CAPE-OPEN Laboratories Network (<u>CO-LaN</u>) is the internationally recognised, user-driven organisation for the management of the CAPE-OPEN (CO) standards. CAPE-OPEN defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate.



The primary purpose of CO-LaN is to promote the use and the development of the CAPE-OPEN standards in Computer-Aided Process Engineering (CAPE) software, and more generally to encourage all actions aimed at facilitating the use of CAPE software tools in industry, government agencies and academia. CO-LaN also helps to facilitate implementation of CO standard interfaces in commercial software to make open simulation a practical reality. CO-LaN main activities are:

- 1. User priorities definition for CAPE-OPEN standards: work with software vendors to clarify user priorities for process modelling software component/environment interoperability and promote use of the CAPE-OPEN standards to create commercially-valuable interoperability;
- 2. Exploitation and dissemination: promote the CAPE-OPEN standards to end-users and distribute CAPE-OPEN information and technology internationally;
- 3. CAPE-OPEN specifications life cycle management: organise the maintenance, evolution, and expansion of the specifications following user priorities;
- 4. Testing, interoperability facilitation: supply compliance testers to support development of components, organise interoperability tests between suppliers of Process Modelling Components and Process Modelling Environments;
- 5. Training/Migration facilitation: ensure that training modules, guidelines and tools to facilitate component wrapping are developed and available.

CO-LaN is a not-for-profit membership corporation. The basis of membership is a Member's interest in the goals and values of the Society. Membership is organised in two categories: Full Members and Associate Members. Full Members are industrial users of CAPE software. Associate Members are providers of CAPE software, government agencies, academic institutions carrying out research activities in the field of CAPE, and other interested parties.

Currently CO-LaN has seven Full Members (Air Liquide, BASF, BP, DOW, Shell, IFP, TOTAL) and thirty two Associate Members including AspenTech, Process Systems Enterprise, ProSim SA, SimSci-Esscor, HTRI, Cosmologic, InfoChem, RSI, Virtual Materials Group and many others including academic institutions such as Carnegie Mellon University, RWTH-Aachen and Denmark Technical University or government agencies such as the US Environmental Protection Agency and the National Energy Technology Laboratory from the US Department Of Energy. Members are currently active through three Special Interest Groups targeted at parts of the CAPE-OPEN standards: Interoperability, Unit and Thermo. These SIGs respectively: insure that software component interoperability issues are resolved (through updating the standards or identifying component design/operation issues); support the ongoing development and expansion of the Unit (operations) standard; support the ongoing development and expansion of the Thermo(dynamics) standard.

To be included in the CO-LaN mailing list, just email a subscribe message to Michel Pons, CO-LaN Chief Technology Officer.

# **Communications**

## Are Recent Graduates Prepared for the Workplace?

by Karl Schnelle, CAST Director

The World Chemical Engineering Council (WCEC) published in September of last year the results of their survey of over 2000 Chemical Engineers. They focused on recent graduates from around the world who entered employment less than five years ago. Questions were asked about general skills and abilities leading to professional employment.

Two results are striking. The first finding is that most recent graduates do not find their first job predominantly in the chemical or petrochemical sectors but in over 27 different industries. Secondly, a disconnect exists between skills needed for employment and those attained in school. These skills are listed as missing from the educational experience: business and management skills, project management, methods for quality assurance, ability to communicate effectively, knowledge of marketing principles, and ethics and professional responsibilities.

The most recent issue of <u>CEP</u> (March 2005, pp 4-6) reports on their findings. Both a summary and full report of the <u>results</u> are also published by WCEC.

#### WebCAST Update

#### by Karl Schnelle, CAST Director

The term *groupware* was coined around 1980 to represent computer technology used for group collaboration, such as software for newsgroups and email listservs, email, videoconferencing, or chat. This collaborative work group technology can be clasified by time: in realtime (synchronous) or at different times (asynchronous), and by location: in the same place (face-to-face) or in different places (distance) (Groupware: Introduction, 11 Mar 2005). Many of you may already use groupware, but CAST has not been an active participant until now. We do actively use mailing lists but only for one-way communication to members.

Now, CAST has taken the plunge into groupware. Last year, we introduced the webCAST as a means to communicate interactively with the membership on specific technical topics. WebCAST is a synchronous, distance-based collaborative conferencing tool. Our implementation uses a regular teleconference phone line for voice and an external internet website for PowerPoint slides or other presentation material. To roll out the webCAST concept took a group effort: Frank Doyle (WebCAST Chair), Vince Grassi (Past CAST Chair), Dan Sliva (AICHE <u>CCPS</u> consultant), and myself.

More details of the 2004 webCASTS are here. We have invited four more speakers for webCASTs in 2005:

- Prof. Michael Doherty, UC Santa Barbara, "Crystal Engineering for Product & Process Design"
- Prof. Costas Spanos, <u>UC Berkeley</u>, "Coping with Variability in Semiconductor Manufacturing"
- Dr. Thomas Sonderman, AMD, "Automated Precision Manufacturing: A Key to Yield in Semiconductor Manufacturing"

• Prof. Sigurd Skogestad, Norwegian University of Science and Technology, "Self-optimizing Control: From Key Performance Indicators to Control of Biological Systems"

If you have other ideas for this year, please let any member of the Executive Committee know.

#### **More Pictures from Austin**

by B. Wayne Bequette, CAST Division First Vice-Chair



Vipin Gopal, Wayne Bequette, unknown, Paul Barton



Juergen Hahn, Eric Hazeltine



Babu Joseph, Jhuma Sadhukhan



Angelo Lucia, Ross Taylor



Tom Marlin, Jim Rawlings



Rakesh Agarwal, Martha Gallivan



Lealon Martin, Raghunathan Rengaswamy



Jeff Siirola, Mike Cutlip, Ms. Siirola

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	Volunteer & Membership Activities
(212) 591-7950	(212) 591-7478
Sarah Fewster	Steve Smith
	Director of Technical Activities & Journals
212.591.7527	(212) 591-7335

#### CAST10 E-Mail List

The following items are used to participate in the list:

- 1. To post messages to the list, please send mail to cast10@ench.umd.edu.
- 2. Subscribe/unsubscribe messages should be mailed to emailman@ench.umd.edu.
- 3. Archived messages can be found at www.ench.umd.edu/cast10.
- 4. Specific instructions on (un)subscribing and posting messages are located at www.ench.umd.edu/cast10/subscribe.shtml.
- 5. Include keywords as the first line of your message: **Keywords: software, jobs, education, meetings** using any or all of the keywords.

The list moderator, <u>adomaiti@Glue.umd.edu</u>, would like to invite comments on the operation of the e-mail list and archive website, especially suggestions for new services.

#### 2005 Award Nomination Form

<sup>Am</sup>The <u>2005 Award Nomination Form</u> [16KB, PDF] should be completed by April 15. See <u>CAST Division Awards</u> for more information.

#### Quote of the Day

"But to everyone, in whatever state of life he finds himself, the ethics of reverence for life do this: they force him without cessation to be concerned at heart with all the human destinies and all the other life-destinies which are going through their life-course around him, and to give himself, as man, to the man who needs a fellow man. They will not allow the scholar to live only for his learning, even if his learning makes him very useful, nor the artist to live only for his art, even if by means of it he gives something to many. They do not allow the very busy man to think that with his professional activities he has fulfilled every demand upon him. They demand from all that they devote a portion of their life to their fellows."

The Philosophy of Civilization Albert Schweitzer (originally published in 1923)

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Already a member? Please ask a colleague to join.

The Computing and Systems Technology (CAST) Division of AIChE is responsible for the wide range of activities within AIChE that involve the application of computers and mathematics to chemical engineering problems including process design, process control, operations, and applied mathematics. We arrange technical sessions at AIChE Meetings, organize special conferences, and publish this newsletter - *CAST Communications* - twice a year. These activities enable our members to keep abreast of the rapidly changing fields of computing and system technology. The cost is \$10 per year, and includes a subscription to this newsletter. Shouldn't you join the CAST Division now?

To join the CAST Division, please contact AIChE Customer Service at the above address. You may also download and print <u>Join a Division or</u> <u>Forum -- Membership Application</u> [30 KB, PDF] from <u>AIChE</u>.

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