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CAST Communications - Special Issue on IT, 2004

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CAST Approves Area 10e on Information Technology

by Jim Davis, UCLA

The CAST Executive Committee has unanimously approved the formation of Area 10e, Information Technology in Chemical Engineering. Formal approval by AIChE is anticipated. [Ed.: Formal approval was granted by AIChE on 18 June 2004.]

Coordinated with and complementary to the other CAST program areas, CAST 10e takes a 'horizontal' systems view of chemical process industry engineering practice, education and research in a networked economy. It is fundamentally about how wired and wireless networks, computation and information technology tools, and social and business practice combine to form new solutions and new businesses in the process industry to increase efficiency and productivity. Program priorities include:

- IT literacy and education,
- interconnectivity and collaboration, where IT enables business objectives,
- 'smart' plant technologies,
- cyber infrastructure technologies,
- infrastructure and frontier technologies,
- new business practices,
- open architectures and
- standards.

CAST10e will emphasize how information technology provides the vehicle for external and internal exchange and contribution. It will concentrate on defining the enabling infrastructure, education and practice required for business-to-client and business-to-business transformation, product customization and choice, manufacturing and product agility, improved operations and reduced risks, multi-company processes and addressing frontier technologies. The viewpoint will be on an IT enterprise that integrates and leverages products and services that are accessible as a single system to meet unique and collaborative requirements for satisfying the needs of customers and stakeholders.

The new program area will be a forum for investigating social and technological change that is facilitated by information technology. Business, manufacturing, research and education in an information technology-enabled environment are increasingly interconnected, collaborative, complex, heterogeneous and distributed. Aggregation, compilation, exchange and study of enormous amounts of data and information across broadly distributed sources have become critical capabilities. Integrating computational tasks of numerical simulation, data analysis and mining, computational steering, distance learning and data exchange are important to emerging practice. Multimedia composition, 3D immersive environments and distributed multimedia computing environments are playing cross cutting roles. Thus, Chemical Engineers are working in increasingly diverse interdisciplinary environments.

CAST10e builds on positive experiences with two topical conferences in Spring 2003 and 2004 and with a special session on information technology in Fall 2003. Programming will kick off with Jim Davis, UCLA, interim program coordinator and topical conference co-chair; and with John Forgac, BP-Amoco and Jimmy Humphrey, Humphrey Associates, interim co-coordinators and

topical conference co-chairs. Upon formal AIChE approval of the new programming area, Jim, Jimmy and John have all agreed to be co-Program Coordinators for 2004 and 2005. CAST10e has set in motion plans to collaborate not only with other CAST program areas but also other divisions in AIChE.

Programming as CAST10e will begin at the Fall 2004 Annual Meeting in Austin on November 7–12, 2004. Those interested in presenting a paper or in participating should contact the appropriate session chairs no later than Tuesday June 1, 2004. Please see the program [pdf, 126KB] for the Topical Conference on Information Technology. For other information on the CAST10e program or the upcoming Topical Conference at Austin, please do not hesitate to contact the Program Coordinators.

Editors' Note: Parts I and II below include IT papers and presentations given at the recent AIChE Spring 2004 National Meeting in New Orleans. And don't miss the Quote of the Day - to find out if you too are a *Bobo* in this new Information Age.

Latest News - *How Much Does Information Technology Matter?*

After writing an article last year entitled "IT Doesn't Matter" for the Harvard Business Review, Nicholas Carr has written a new book, *Does IT Matter?*. Varian writes: "Mr. Carr lays out the simple truths of the economics of information technology in a lucid way, with cogent examples and clear analysis. ... At one time, information technology was so expensive and so difficult to manage that companies could make large amounts of money simply by being able to make systems work." But now, Carr argues that IT has become a utility and not a source of competitive advantage; everyone knows how to set up a web server, implement an information management system, etc. "It is not information technology itself that matters, but how you use it."
(Hal R. Varian, The New York Times, 6 May 2004)

And a Rebuttal - *The Engine That Drives Success*

"The best companies have the best business models because they have the best IT strategies. ... Market leaders grab positional advantage through a combination of IT and business design, and then others have no choice but to follow in their wake."
(Don Tapscott, CIO Magazine, 1 May 2004)

Part I. Enterprise-Wide Optimization

How chemical engineers can take advantage of integrated strategic, tactical and operational decision-making to optimize customer engagement, manufacturing, supply chain and financial processes.

An Overview of Enterprise-Wide Optimization Presentation [296 KB]
by Vince Grassi, Andy Bringhurst, Ken Anselmo, Tom Brinker, Jim Hutton; Air Products & Chemicals, Inc.

These papers will provide an overview of Enterprise-Wide Optimization (EWO), the business areas that are impacted by this approach, and the associated interactions between the required decision models. This presentation will also discuss how the widespread implementation of Enterprise Resource Planning (ERP) has created new opportunities for implementing EWO strategies. Finally, we will indicate how the other presentations in Part I fit into the overall EWO landscape.

The presentation [296 KB] may be downloaded in pdf format.

Managing Supply Chain and Operational Crisis Using Scheduling Algorithm for Overall Refinery Operations Presentation [735 KB]
by Dhaval Dave and Nan Zhang, UMIST

An objective common to all refiners is to improve profitability by improving their operating strategies. Planning tools for making long-term decisions are available to almost all the refiners. The profit of a refinery now a day depends upon how they respond to crisis-making situations and dynamic market conditions. It is very important to exploit short-term market opportunities such as low-cost availability of crude-oil as well as opportunities for selling high valued products as much as possible. Also, profit loss during emergency situations should be minimised. In the present work, scheduling model has been developed for such decision making and capabilities are demonstrated using various case-studies.

Firstly, detailed mathematical models of information, raw material and product flows in the refinery have been developed. Crude oil and feedstock procurement retrieves crude availability posting from the market and decides which oil to purchase and in what amount. Next, logistics department arranges the transport of crude from the oil supplier terminal to the refinery. Generally, transportation is done by the third party and transportation cost is a function of size of cargo and distance. For the cases, where crude oil and products are transported by shipment, marine tank farm manages schedules of oil and product jetties. It ensures that the customer demand is satisfied and the refinery gets the required supply of crude-oil on regular basis. Refinery tank farm stores, blends and processes crude oil, intermediate and final products. Refinery processing department decides which blend to charge and how much to process everyday. It also decides various operating conditions for the refining process. It has been assumed that refinery management receives information from all the departments regularly and makes the decisions.

Since a refinery involves many non-linear process models, mixers, splitters etc., optimisation of overall refinery scheduling problem becomes a large scale mixed integer nonlinear programming (MINLP) problem. A decomposition method has been proposed to separate economically important mixed integer linear programming problem from nonlinear process aspects. Developed MILP and NLP recursive technique was able to generate good quality schedules with in practical computational time.

Next, several case-studies are demonstrated for utilising developed scheduling software for making supply chain and crisis-time decisions. Various scenarios studied are selling or purchasing crude oil cargoes depending upon market conditions, to evaluate opportunity to meet short-term product demands and what-if studies for unplanned unit shut down. Decision making for buying or selling a cargo is very difficult. For example, refiners purchase low cost crude oil then risk of running unstable operations exists. On the other hand, if they do not purchase the crude oil an opportunity has been lost in order to save on raw-material cost. Scheduling software evaluates such short-term opportunities considering refinery topology and operating strategies. Same kind of case-studies performed for evaluating short-term product demands and to decide the earliest and latest delivery due dates. And finally, various operational disturbances such as unplanned unit shutdown are considered and profit-loss during such situations minimised using developed scheduling software.

The presentation [zip, 735 KB] or presentation [pdf, 1.6 MB] may be downloaded.

Optimization Based Approach for Managing Enterprise-Wide Business Planning in a Petrochemical Industry

Presentation [2.7 MB]

by Bhieng Tjoa and Arturo Cervantes, Optience Corp.; and Kagoto Nakagawa, Mitsubishi Chemical Corp.

Business planning for an integrated petrochemical company is fairly complex and challenging problem. The manufacturing resources typically start with a co-products continuous plant which has flexibility of processing various types of feedstock. Some products from this upstream plant may be directly used as feedstock for other downstream plants. Each of these downstream plants may produce various products in continuous or batch operations. In such integrated business, planning activity is very important to ensure that the overall profitability of the company is optimized. The opportunity for improving profitability can be significant, and it is both process and market dependence.

Here, we discuss issues that are important in addressing the enterprise wide planning problem, from data requirement and management to modeling and optimization. We propose an optimization based application environment that is database centric. It utilizes a visual task based modeling approach for building a multi-plants and multi-sites supply chain planning problem as one optimization model. The mathematical programming model representation is automatically generated and optimized during the execution to find the best possible solution. The system supports a wide range of optimization problems from simple Linear Programming (LP) to Mixed Integer Nonlinear Programming (MINLP) models. This approach will be demonstrated on an ethylene and its derivative business.

The presentation [2.7 MB] may be downloaded in pdf format.

Achieving Lowest-cost Emission Level Compliance under Cap & Trade Using a Math Programming-based Emissions Optimizer that Links Regional Customers through a Web-based Environmental Management Information System

Presentation [710 KB]

by Derrick Schertz and Joseph Pekny, Advanced Process Combinatorics, Inc.; Richard McAllister, Beth Brandes Jenkins, Bruce Snyder, Semra Alici, Edward Galligan, Carlos Valenzuela, and Mark Daichendt, Air Products & Chemicals, Inc.

The Houston-Galveston Area (HGA) is classified as a "serious" ozone non-attainment area. Over 2750 point sources are subject to treatment to reduce NOx emission levels (ton/year) by 80%. Based on current point source activity levels (MMBTU/hr) and emission factors (lb NOx/MMBTU), each company must achieve specific NOx emission level limitations, staged between 2003 and 2008. Various treatment technologies are available for the different types and sizes of units. These technologies have different capabilities (lb NOx/MMBTU) and investment costs ($-hr/MMBTU). In many cases, two technologies can be combined.

Air Products & Chemicals, Inc. (APCI) had conceived a unique Services & Solutions e-Business offering, which would establish a proprietary web-based Environmental Management Information System to integrate data from the Texas Commission on Environmental Quality (TCEQ) and the customers' forecasted point source emission levels to provide input to an Emissions Optimizer (EO). Air Products has applied for a patent to protect this business model. The model is configured to handle any type of emission data and non-attainment geography.

APCI and VisionMonitor Software LLC entered into an alliance partnership to develop the VisionMonitor Compliance Intelligence (CI) solution. The CI solution enables organizations to track, monitor and predict their compliance with various regulatory standards and reporting requirements across the enterprise. Additionally, the CI solution provides the link between the participating customers in the affected region and EO.

The selection of the lowest cost of compliance for the entire HGA involves discrete decisions. These are, for each point source, when to install what remediation technology or combination of technologies over a six-year time horizon. These discrete decisions are represented by integer (0/1) variables. The lowest-cost solution to this question can be found by formulating a Mixed-Integer Linear Programming (MILP) problem.

Large-scale MILPs are considered intractable, because the number of potential solutions to an MILP problem grows exponentially with the number of integer variables. While there is no known algorithm that can solve general MILP problems in polynomial time, previous projects with Advanced Process Combinatorics, Inc. (APC), a venture spin-off company from Purdue University, had shown that, through careful problem formulation, decomposition techniques could be applied to exploit problem structure, and algorithms could be engineered to solve the specific class of problem under consideration.

APCI's EO was developed in collaboration with APC using the latter's VirtECS Design tool. The model parameter input database and basic structure of the NOx problem were developed at APCI. APC created a customized NOx Model Manager and then tailored the problem formulation and solution algorithm to perform the optimization in an acceptable amount of time using their proprietary VirtECS solver technology. The NOx Model Manager generates the desired results for transfer back to the database.

The EO determines the lowest cost of compliance with the Texas State Implementation Plan. First, an enterprise-wide optimization is performed for each company. This is followed by a regional optimization for all participating companies acting as a consortium. The optimization determines at each time period which companies should over-control their point sources to what extent to generate and sell credits, and which companies should under-control their point sources to what extent and buy credits.

Trading is implicit in the MILP framework, so a subsequent Nonlinear Programming (NLP) optimization is performed based on the MILP results to determine the ton per year (TPY) and dollar exchanges corresponding to the Cap & Trade program. This NOx Trading Model was developed at APCI using the Generalized Algebraic Modeling System (GAMS).

The difference in capital investment between the two solutions forms the economic basis for determining the marginal values between the buyers and sellers ($/TPY). The difference in the marginal values provides the driving force for trades, and the net savings between the two MILP solutions is partitioned between the sellers and buyers. The NLP trading model essentially maximizes the area between the two curves, corresponding to the net capital savings, in such a way that the sellers receive more revenue than their additional investment required to generate credits, and buyers pay less through credit purchases than their alternative to invest in additional equipment.

These models have been solved for the entirety of the point sources belonging to all the companies in the HGA. Activity level and emission factors were taken at the base-values from the TCEQ database. Marketing reports and internal studies were used to generate appropriate treatment technology options, capabilities, and costs for each point source. The VisionMonitor CI solution returns the enterprise-wide EO solution directly to the customer. APCI's sales team follows up with a benefits opportunity analysis to those companies that can achieve a significant cost savings through trading.

The EO is a key differentiating component of APCI's compliance monitoring and optimization product. The EO provides a successful example of how technical advances made by academic researchers can be transformed into viable commercial products, and, by cultivating a long-term industrial-academic relationship, changing business needs can be used to identify new opportunities to advantageously apply optimization technology to determine solutions to critical problems.

The presentation [710 KB] may be downloaded in pdf format.

Optimization of Operations in an Enterprise Presentation [2.4 MB]
by V. Mahalec, M. Chevis, and D. Clark; Aspen Technology

Over the last two decades, process industries have implemented numerous IT systems that aim to improve decision making in all aspects of enterprise operations, from finance to feedstock supply, to manufacturing, to product distribution, to plant maintenance and design. In parallel, advances in software technology have made it possible to integrate individual applications to support all aspects of information analysis and decision-making for a given business role.

Hence, the industry is at the dawn of an era of ever increasing accuracy and agility in decision-making. Business processes that decide what is the best course of action and then execute the corresponding actions are referred to as Enterprise Operations Management. Such processes are be enabled by models of enterprise capabilities (accuracy), integration of business processes (agility), and real-time implementation of decisions.

AspenTech provides solutions for supply chain planning, scheduling, inventory management, manufacturing, and facility planning or improvement via process design. These solutions enable enterprises in process industries to move from installed base of individual solutions to integrated solutions. Implementation of these solutions is facilitated by a standard deployment environment (“Operations Manager”) that enables decision-making at different levels in the organization, and by the AspenTech’s decision support models (e.g. planning, scheduling, process optimization, optimal design, etc.).

The paper will describe AspenTech’s vision for Enterprise Operations Management, progress in delivery of the solutions, and an evolutionary path that will enable process industry to move to a qualitatively new level of optimal decision making across the enterprise.

The presentation [zip, 2.4 MB] or presentation [pdf, 5.8 MB] may be downloaded.

Part II. Lessons Learned in Information Technology

How you can leverage lessons learned and examples of best practices in manufacturing and business process improvement.

Today's Technology for Operational Excellence - Best Practices in Manufacturing
by Steve Williams, Aspen Technology

Article [478 KB]
Presentation [3.8 MB]

This paper considers the role of newly emerging technologies in supporting Operational Excellence particularly in the areas of:

- Integration infrastructure for bringing together diverse data in manufacturing environments
- Improved visibility (web-based views of real-time information)
- Event management for intelligent alerting and automated responses to important business events
- Peformance Scorecarding and Analytics (for making performance versus target very visible and providing the analysis environment to understand and improve performance
- Look Ahead Analytics for projecting future performance and improving future profitability (not just learning from past performance)

The paper incorporates application examples at customer sites.

The full article [pdf, 478 KB] and the presentation [zip, 3.8 MB] or presentation [pdf, 6.7 MB] may be downloaded.

Solutions for Successful Chemical Inventory Management
by Marc Dillon and Dawn Kehr, ESS

Article [135 KB]
Presentation [141 KB]

Chemical inventory management, as it relates to environmental, health and safety professionals, essentially consists of the following components:

- Chemical purchases and receipts
- Chemical inventory transactions (storage and use)
- Inventory Management
- Record keeping
- Reporting

These five elements comprise the chemical inventory management life cycle: from when chemicals are ordered, purchased and received at the facility, to when they are stored, used and depleted for disposal. Inventory management includes tracking and maintaining proper inventory levels to maintain production or other important operational processes. Record keeping includes maintaining accurate records of the previous elements and up-to-date Material Safety Data Sheets (MSDSs) for the chemicals in inventory. All these data are used for creating reports including SARA 312 Tier I or Tier II, and permit required reports that may include hazardous air pollutant (HAP) and volatile organic compound (VOC) usage data.

This paper will review the types of software products that are available to assist EH&S professionals manage, automate, and improve their overall regulatory-compliance in regard to chemical inventory processes. Recommendations will be provided about when certain types of software products might be used and several key issues and questions will be addressed to assist chemical process engineers evaluate potential chemical inventory management software vendors.

The full article [135 KB] and the presentation [141 KB] may be downloaded in pdf format.

Best Practices in Alarm Management - Experience from the Field
by Nadya Dhalla, Matrikon Inc.

Article [103 KB]
Presentation [1.2 MB]

Effective safety systems are a fundamental requirement of industrial facilities today. Matrikon Inc and an Operating Company will discuss best practices in alarm and event management. The Operating Company will share operational experience at their x facilities world wide has provided a basis for their Best Practice program on Alarm Management. Matrikon's experience implementing ProcessGuard - Alarm Management technology, at over 100 facilities world-wide has also provided an experience base to draw upon for best practices - offering some cross-industry analysis.

The full article [103 KB] and the presentation [1.2 MB] may be downloaded in pdf format.

Cutting the Wire. Real Life Experiences About Going Wireless - Emerging Digital Technology
by David Hrivnak, Eastman Chemical Company

Article [243 KB]
Presentation [931 KB]

This paper and presentation will give an overview of wireless technologies and how they can be used to improve operations and lower cost in the chemical industry. David Hrivnak, Mobile Projects Manager, will discuss three broad areas of wireless technology. He will discuss what Eastman did and what they have learned through the deployments.

- Wireless LAN technology & security and our worldwide deployment.
- Wireless WAN & how Eastman provides workers with wireless e-mail when on the road
- Wireless Sensors and how we have begun to test and deploy this new technology.

The full article [243 KB] and presentation [931 KB] may be downloaded in pdf format.

Organizational Considerations for Implementing IT Applications Presentation [418 KB]
by Gary Stenerson, ExxonMobil

When developing IT applications, implementation planning should consider several aspects of how the application affects the people involved. This paper explores how project planning should recognize the affects of human nature and the interaction with the application in developing and implementing IT applications by:

- Developing a thorough change management plan
- Establishing a detailed set of business requirements for the overall business process(es) being affected, in addition to those being automated/optimized by the application
- Integrating work and data flows into the overall business process(es)

The presentation [zip, 418 KB] may be downloaded in pdf format.

The After Action Review - A Lessons Learned Process Presentation [567 KB]
by Vince Grassi, Air Products & Chemicals, Inc.

The After Action Review is a formal process for the collection and dissemination of lessons learned. The After Action Review process was developed by the United States military as a way to quickly capture what was learned after an event. The process is easy to remember, quickly apply, and easy to communicate the results to others that can take action on what was learned.

Air Products has used this process and a method to capture the lessons learned in a call center repository so that they can be adapted across the enterprise.

This presentation will present the method, give examples, and explain the key success factors on how you can apply the method in your organization. Participants will leave this session able to use After Action Reviews to capture and take action from lessons learned sessions.

The presentation [567 KB] may be downloaded in pdf format.

Quote of the Day

"In this era ideas and knowledge are at least as vital to economic success as natural resources and finance capital. The intangible world of information merges with the material world of money, and new phrases that combine the two, such as 'intellectual capital and 'the culture industry,' come into vogue. So the people who thrive in this period are the ones who can turn ideas and emotions into products. These are highly educated folk who have one foot in the bohemian world of creativity and another foot in the bourgeois realm of ambition and worldly success. The members of the new information age elite are bourgeois bohemians. Or, to take the first two letters of each word, they are Bobos.

"These Bobos define our age. They are the new establishment. Their hybrid culture is the atmosphere we all breathe. Their status codes now govern social life. Their moral codes give structure to our personal lives...

Bobos in Paradise: The New Upper Class and How They Got There
David Brooks, 2001

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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 Join a Division or Forum -- Membership Application [30 KB, PDF] from AIChE.

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