This column addresses aspects of lifelong learning for current students, alumni, and faculty. Examples of student and faculty activities that involve industrial practice and engagement as well as continuing education are welcome. These topics may not always lend themselves to the traditional scholarly format with formal assessment and extensive literature review but may be more editorial in nature. Please submit manuscripts to Professor Lisa Bullard at lisa_bullard@ncsu.edu

THE CENTER FOR ADVANCED PROCESS DECISION-MAKING AT CARNEGIE MELLON

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For almost half a century, Process Systems Engineering (PSE) has been a strong research pillar in the Chemical Engineering Department at Carnegie Mellon University. In 1985, we formed the Center for Advanced Process Decision-making (CAPD) to further advance PSE research and guide fundamental research to practical applications. Now an internationally recognized research leader in computer-aided process systems engineering, the CAPD is engaged in systems engineering research for the process industries. With support from the National Science Foundation, the Department of Energy, member companies, and other funding agencies, the CAPD group has pioneered the discovery, development, and application of new methods for process design, analysis, and operations. Our research goals are to understand complex design and operation issues faced by industry, and to develop and advance modeling and solution methods for process systems engineering. General information on the CAPD can be found in <http://capd.cheme.cmu.edu>.

The CAPD is a unique research group that deals with the development of methodologies and computational tools for the process industries. The CAPD consortium currently has more than 20 members from the chemical and petroleum industries as well as a number of services and software companies. CAPD's research work is directed by Professors Biegler, Gounaris, Grossmann, Sahinidis, and Ydstie, and is carried out by more than 70 graduate students and researchers from the Department of Chemical Engineering. Its main areas of research include modeling and simulation, process synthesis, process optimization, process control, scheduling and planning, supply chain management, energy systems,

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Ignacio Grossmann *is the Dean University Professor of Chemical Engineering, and former department head at Carnegie Mellon University. He obtained his B.S. degree at the Universidad Iberoamericana, Mexico City, in 1974, and his M.S. and Ph.D. at Imperial College in 1975 and 1977, respectively. He is former director (2005-2015) of the Center for Advanced Process Decision-making. He has authored several monographs on design cases studies, and the textbook* Systematic Methods of Chemical Process Design, *with Larry Biegler and Art Westerberg. He has also organized the Virtual Library on Process Systems Engineering.*

Nick Sahinidis *is the John E. Swearingen Professor and director of the Center for Advanced Process Decision-making at Carnegie Mellon University. He joined Carnegie Mellon in 2007 after a 16-year career at the University of Illinois at Urbana. His research has included the development of theory, algorithms, and the BARON software for global optimization of mixed-integer nonlinear programs. His research activities have been recognized by the Computing in Chemical Engineering Award in 2010, the Constantin Carathéodory Prize in 2015, and the National Award and Gold Medal from the Hellenic Operational Research Society in 2016, among others.*

molecular design, bioinformatics, and data analysis. Most importantly, our main mission is to train future researchers and educators in the PSE field. To this end, the CAPD promotes interactions in industry related to PSE research, offers short courses for researchers and practitioners, and produces textbooks, monographs, software, and educational tools that advance the field.

HISTORY OF THE CAPD

Since the 1960s, Carnegie Mellon University has spearheaded the advancement of systems concepts in all areas of science and technology. Carnegie Mellon's engineering faculty have been instrumental in catalyzing revolutionary changes resulting from the introduction of computer and systems technology to science and industry. In process systems engineering, Carnegie Mellon's effort began in the mid-'70s with the creation of the Design Research Center (DRC). This interdisciplinary group saw significant participation by chemical engineers (Gary Powers, Art Westerberg, Ignacio Grossmann, and Larry Biegler) and led to the development of core systems methodologies for process engineering, including optimization algorithms and formulations, operations research methods, artificial intelligence, expert systems, and software engineering.

With the award of Presidential Young Investigator grants to Grossmann and Biegler in the mid-'80s, there was a strong motivation to attract industrial collaboration and support through matching research funds. Together with the active participation of Art Westerberg, a strong effort began to create a cohesive research group in process systems engineering. At the same time, the DRC expanded to an NSF-sponsored Engineering Research Center, called the Engineering Design Research Center (EDRC), which was funded from 1985 to 1996, before transforming into the Institute for Complex Engineered Systems (ICES), an integral part of CMU's College of Engineering.

With support from the National Science Foundation, the Department of Energy, and the process industries, our group has pioneered the discovery, development, and application of new methods for process design, analysis, and operations. A summary of milestones since the founding of the CAPD consortium can be found in <http://capd.cheme.cmu.edu/history_pse.html>. Currently, our research activities combine strong systems science components and industrial interactions in the areas of process synthesis and analysis, process operations, molecular modeling, and data analysis.

As a result of this growth, the CAPD captures a broad range of areas in Process Systems Engineering that extends far beyond traditional chemical process design. With the addition of Erik Ydstie in 1992, process control became a focus research area. The addition of Nick Sahinidis in 2007 and Chrysanthos Gounaris in 2013 brought further strengths in core optimization areas, as well as new applications at the molecular level (X-ray imaging, bioinformatics, and molecular and materials design). Moreover, the CAPD enjoys a long association with Jeff Siirola, who provides experienced guidance in conceptual design of chemical and energy processes, served as distinguished service professor from 2011 to 2017, and continues to teach the process synthesis part of the CAPD short course. As a result, research efforts within the CAPD have led to a multitude of strategies and tools for process design and operations for both batch and continuous processes. These include:

- *mathematical programming software tools that are widely adopted in free and commercial forms;*
- *design strategies for process synthesis;*
- *advanced modeling environments for process modeling and optimization;*
- *optimization platforms for planning, scheduling and supply chain management*

A sampling of topical research areas and applications is presented in Table 1.

INDUSTRIAL INTERACTIONS

In addition to federal and state funding sources, research in the CAPD has been supported by more than 20 industrial member companies; the current list of members is presented in Table 2. Member companies participate in the CAPD through a broad array of activities. They initiate PSE projects in their domains of interest, sponsor graduate students, provide industrial internships related to PSE projects, interact on long-term research that advances the field of PSE, and provide employment opportunities for our M.S. and Ph.D. students and postdocs.

Many of our member companies participate in our two special interest groups: Enterprise-wide Optimization (EWO) and Energy Systems Initiative (ESI), which include specific projects in these areas as well as seminars on a variety of related topics. The goal of the EWO group is to provide a comprehensive set of computational capabilities for addressing the integrated planning, scheduling, real-time optimization, and inventory control of process systems. Companies who currently participate in the EWO group include ABB, Air Liquide, Aurubis, Braskem, Covestro, Dow Chemical, ExxonMobil, Ecopetrol, EQT, Mitsubishi Electric, Petrobras, P&G, Praxair, Sabic, SK Innovation, and Total. These companies typically supply case-study projects that are undertaken by PSE faculty and students. More recently, the CAPD has developed close collaborations with the National Energy Technology Laboratory (NETL), which has led to a number of projects related to modeling, optimization, and control for energy systems. The Energy Systems Initiative (ESI) comprises projects related to energy systems, and includes topics ranging from solar cell research to technologies for CO_2 capture and sequestration, and advances in energy efficient

systems. For more details on the EWO and ESI groups, the reader is referred to <http://egon.cheme.cmu.edu/ewo/> and <http://egon.cheme.cmu.edu/esi/>.

Throughout the years, interactions between CAPD researchers and industry have led to numerous success stories. For instance, in his 2017 presentation at the FOCAPO (Foundations of Computer Aided Process Operations) conference, Shawn Feist of The Dow Chemical Company described Dow's University Partnership Program, an innovative partnership between Dow and a dozen universities. Dow's partnership with the CAPD was singled out as an exceptional program that resulted in multimillion dollar annual savings for Dow through CAPD's novel algorithms for real-time optimization of polymers and for scheduling multibillion-dollar turnarounds of interacting industrial complexes.

In addition to research interactions, all member companies receive reports, papers, and relevant software resulting from the consortium's research. Members also participate in annual review meetings, held every spring in Pittsburgh, to discuss ongoing projects with academic staff, students, and fellow members. Meetings consist of overviews given by the faculty, presentations and discussions by industrial participants, and a poster session as well as final-year student presentations. Finally, every year, members send several of their employees to participate in our seven-day short course on modeling, optimization, and integrated process operations.

TABLE 1
Research areas

Modeling and optimization algorithms	Modeling, simulation, and control of distributed systems
	Large-scale nonlinear programming
	Optimization of differential-algebraic systems
	Mixed-integer programming, disjunctive programming
	Global optimization
	Stochastic programming
Process synthesis	Synthesis of heat exchanger networks
	Synthesis of integrated process flowsheets
	Synthesis of complex separation systems
	Synthesis of integrated process water systems
Enterprise-wide optimization and process operations	Scheduling and planning of batch and continuous process systems
	Production scheduling and distribution logistics
	Enterprise-wide optimization and supply chain management
	Thermodynamics-based process control
	Optimization strategies for process control and parameter estimation
	Verification of control system software and human operating procedures
Product design and molecular computing	Design of environmentally benign molecules and mixtures
	X-ray crystallographic computing
	Molecular structure prediction
	Structural biology
	Design of microporous materials
	Design of solvents
	Analysis and design of metabolic networks
Energy systems	Synthesis and design of energy intensive processes
	Design of energy and shale gas systems
	Design of oil and gas offshore infrastructures
	Modeling and risk assessment of CO_2 sequestration
	Design and analysis of fuel and solar cells
	Demand-side management
	Planning of electric power systems
Data analytics	Adaptive control and online parameter estimation
	Bioinformatics
	Machine learning
	Reduced-order modeling
	Data analytics methods for stochastic programming

TABLE 2
List of current CAPD members

ABB
AIMMS
Air Liquide
Air Products
Aurubis
Braskem
Covestro
Dow
Ecopetrol
Eastman Chemical Company
EQT Corporation
ExxonMobil
GAMS
Mitsubishi Electric Research Laboratories
Neste Jacobs
National Energy Technology Laboratory
Petrobras
Praxair
P&G
Sabic
SK Innovation
Total

SHORT COURSE—CONCEPTUAL DESIGN, OPTIMIZATION MODELING, AND INTEGRATED PROCESS OPERATIONS

Research in process systems engineering is a complex synthesis of applied mathematics, operations research, and control theory, as well as basic science. Within the CAPD, a key mission is the dissemination and application of our research results among researchers and practitioners, both in academia and in industry. Consequently, an essential mission of the CAPD is the educational component that relates to our research.

Since 1988, the CAPD has offered an annual short course that showcases the strengths of mathematical modeling, design, operations, and optimization approaches in process systems engineering. This course has been offered to advanced researchers, including Ph.D. students, postdocs, and faculty from other universities, as well as industrial practitioners. In the current incarnation of this course, we offer a week-long course entitled "Conceptual Design, Optimization Modeling, and Integrated Process Operations." As described in Table 3, this course is organized in three modules on (1) conceptual design, (2) optimization, and (3) integrated process operations. The course consists of seven self-contained lectures that can be taken altogether or in subsets. Topics include: nonlinear, discrete, and global optimization; conceptual design; and integrated process planning, scheduling, and control.

Each lecture day balances theory, algorithms, and applications. For example, the lectures that make up the optimization module provide:

- *An in-depth discussion of fundamentals (convex analysis and optimality conditions)*
- *Conceptual treatment of algorithms for linear, nonlinear, integer, and nonconvex programming*
- *Broad coverage of many modeling paradigms (discrete/continuous, deterministic/stochastic)*
- *Demonstrations of the application of the theory and algorithms in process systems engineering, including flowsheet synthesis and optimization, as well as optimization of process operations.*

TABLE 3
Organization of CAPD Short Course: conceptual design, optimization modeling, and integrated process operations

Module I. Conceptual design—focuses on creation of superior process concept alternatives • Process synthesis
Module II. Optimization modeling—focuses on modeling and algorithms with applications to process optimization, process synthesis and molecular design: • Nonlinear programming • Mixed-integer and disjunctive programming • Global optimization and optimization under uncertainty
Module III. Integrated process operation—focuses on three major decision levels in plant and enterprise-wide optimization: • Mixed-integer models for planning and scheduling • Advanced process dynamics and control • Differential-algebraic models for real-time optimization

Overall, our short course stresses the application of optimization models and methods to practical process problems and recently developed process synthesis concepts. The course provides practical information and exposure to powerful and sophisticated modeling tools for process synthesis, planning, scheduling and dynamics, and control, including treatment of uncertainty; the transfer of information is facilitated through lectures and hands-on workshops. Course materials include modeling tools and optimization software that incorporates state-of-the-art nonlinear and mixed-integer programming algorithms and models. As a result, the course emphasizes systematic solution approaches and provides the necessary background to understand the tools and apply them correctly and efficiently to process problems.

Typically, our course participants include industrial researchers and engineers, advanced graduate students, and academic researchers from around the world. Most students are chemical engineers. However, the backgrounds of students have included electrical engineers, mechanical engineers, industrial engineers, chemists, and mathematicians. The course has been very successful for: process engineers interested in obtaining improved solutions for design, planning, scheduling, and control problems; researchers interested in quickly testing new process ideas and concepts through the use of optimization-based tools; and managers interested in understanding and introducing advanced PSE tools in their working environments. In addition to offering the course on an annual basis in Pittsburgh, we offer selected subsets of the material at industrial sites that request it.

Testimonials from our past short course participants include:

- *"I liked the combination of theoretical and practical applications of the optimization methods. The rationale behind each technique was also well explained."*
- *"This course helped me to gain a nice perspective on the optimization modeling front."*
- *"All of the (course) modules had elements that fascinated me."*
- *"Thank you for organizing this course and for providing the participants to be a beneficiary of the vast experience and knowledge of the instructors."*

We should also note that educational material on a variety of topics in process systems engineering can be found in the Virtual Library of PSE: <http://cepac.cheme.cmu.edu/pasilectures.htm>.

SUMMARY AND FUTURE OUTLOOK

For more than 30 years, the Center for Advanced Process Decision-making has made major contributions and developed a strong track record toward advancing PSE concepts for the modeling, design, and optimization of improved chemical processes and products. As seen in Table 4, CAPD has strongly

contributed to the education of a large international academic community in process systems engineering. Table 5 illustrates the diversity and quality of the placement of CAPD students in industry. These tables also serve to highlight the CAPD's major accomplishment over the past three decades, namely the production of a very large number of highly successful graduates who have had tremendous impact across several universities and industrial sectors. Some recent graduates and current students and postdoctoral researchers at the CAPD are shown in Figure 1. Participants in the 2017 CAPD Short Course banquet are in Figure 2.

For the future, our goal is the further development of leading-edge research in fundamental systems areas and the application of these results to challenging real-world problems in science and engineering. Our key mission remains to educate the next generation of leaders and practitioners. Towards this end, we have found that there exists a strong interplay between research and teaching that results in the development of high quality educational materials, including lecture material and software that, in turn, catalyze further research advances. ❐

Table 4
Academic alumni of the CAPD

Luke Achenie (VPI)
Rene Bañares (Oxford)
Lisa Bullard (NC State)
Alex Dowling (Notre Dame)
Keshava Halemane (Karnataka NIT)
Andy Hrymak (Western Ontario)
Carl Laird (Purdue)
Jaewoo Lee (KAIST)
Yoshi Kawajiri (GA Tech)
Christos Maravelias (Wisconsin)
Nuno Oliveira (Coimbra)
Joe Pekny (Purdue)
Stratos Pistikopoulos (Texas A&M)
Vicente Rico-Ramirez (Celaya)
Nick Sahinidis (CMU)
Ross Swaney (Wisconsin)
Metin Turkay (Koc)
Andreas Waechter (Northwestern)
Fengqi You (Northwestern)
Juan Zamora (UAM)
Victor Zavala (Wisconsin)

TABLE 5
Placement of CAPD alumni in industry (partial list)

ABB
Abu Dhabi NOC
Air Liquide
Air Products
AkzoNobel
Amazon
Artelys
Aurubis
AspenTech
AT Kearney
Bank of America
Bayer
Bloomberg L.P.
BP
Capital One
Chevron
Dow
DuPont
Eastman Chemical
ExxonMobil
GAMS
Google
IBM
Invensys
KBC
McKinsey
Microsoft Research
Nielsen Marketing Analytics
OSIsoft
Owens
PEMEX
Process Systems Enterprise
Praxair
Quintic
Rockwell Automation
Saudi Aramco
Soteica
Shell
United Technologies

Figure 1, top. *Recent CAPD graduate students and postdoc researchers at Annual Review.*
Figure 2, bottom. *CAPD Short Course banquet participants, 2017.*