CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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<u>Erik Ydstie's Group</u>

GENERAL NEWS

Praxair joins CAPD. We would like to welcome Praxair who has joined CAPD and the special interest group on EWO. The representatives of Praxair are Dr. Jose Pinto, Dr. Larry Meghan and Dr. Nikhil Arora. We very much look forward to the participation of Praxair at the CAPD.

Gary Powers This is to remind you that an undergraduate scholarship has been established in the memory of Gary. Donations may be sent to the Gary J. Powers Scholarship Fund, c/o Toni McIltrot, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15222-5488.

Ignacio Grossmann taught a short course on MINLP optimization and process synthesis at the University of Antofagasta, Chile, in January, 2008. He also gave the talk "Trends in Chemical Engineering Curriculum: a U.S. Perspective", in the Department of Chemical Engineering and Bioprocesses, Catholic University, Santiago de Chile. Ignacio participated in the Symposium on Trends in Chemical Engineering at the Department of Chemical Engineering, Universidad Autonoma Metropolitana-Iztapalapa, Mexico City, where he gave the plenary talk "Research Challenges in Process Systems Engineering and its Potential Impact in the Process Industry." He also gave the seminar "New Developments in Discrete-Continuous Optimization of Process Systems," in the Department of Chemical and Biological Engineering, RPI in March, and in the Department of Chemical Engineering and Biological Engineering, Tufts University in April, 2008. Ignacio also gave a short course on enterprise-wide optimization at INETI in Lisbon, as well as a seminar at the Instituto Superior. He gave the talk "Reformulations, Relaxations and Cutting Planes for Linear Generalized Disjunctive Programming," at the workshop on Hybrid Systems in Istanbul, and at the MIP-2008, Columbia University, New York (2008). Ignacio's group participated at the FOCAPO meeting having a total of 8 contributed papers. Ignacio also participated in the advisory board meetings of the Department of Chemical Engineering at Penn State, of the Institute of Chemical and Engineering Sciences in Singapore, and of Engineering Sciences at Dow Chemical. Finally, Ignacio and Laura organized the Pan American Advanced Studies Institute on Emerging Trends in Process Systems Engineering (see below).

Nick Sahinidis was appointed Faculty Research Fellow of the Institute for Advanced Engineering Solutions at DOE's National Energy Technology Laboratory. He was elected as the chair-elect of the INFORMS Optimization Society and will become chair of the Society in 2009. Nick gave a talk on "Optimization in the New Biology" at Georgia Tech's Center for the Study of Systems Biology, the University of Pittsburgh School of Medicine, CMU's Tepper School of Business, and the Department of Chemical and Biological Engineering at the University of Wisconsin, Madison. He gave a related invited talk "Optimization Techniques in Molecular Structure and Function Elucidation," at *Foundations of Computer-Aided Process Operations 2008,* in July 2008. In March 2008, he gave a plenary talk on Global Optimization at the 5th International Conference on Computational Management Science, Imperial College, London, U.K. In July 2008, Nick was appointed to the editorial board of *Mathematical Programming Computation (MPC).* This new journal is sponsored by the international Mathematical Programming Society and will be a companion to the Society's highly regarded journals *Mathematical Programming Series A and B.*

Erik Ydstie was awarded the 2008 Kun Li Award for Excellence in Education during the graduation ceremony in May. He gave seminars on process systems and networks at the Chemical Engineering departments at Queens University in Canada and University of Maryland. He participated in a due diligence process for a $500M new solar silicon plant in the months of May and June. Erik's students gave papers at the American Control Conference, the IEEE Power conference in Florida, the IEEE power conference in Pittsburgh, the IFAC World Congress in Seoul and the FOCOPO conference in Boston. Erik obtained the "Certificat de Asencion de Machine Aerostatic" in Phoenix in July and participated in the American Chemical Society Advisory Board Meetings in Portland OR in May. He also presented a paper and took part in the review meetings of the Center for Integrated Operations in Trondheim Norway.

Congratulations to **Victor Zavala** for defending his Ph.D. thesis on "Computational Strategies for the Optimal Operation of Large-scale Chemical Process." Victor has accepted a position at the University of

Texas-Austin as an assistant professor. Prior to starting this position, he will be a postdoctoral fellow in the Math and Computer Science Division at Argonne National Laboratory.

Congratulations to **Rui Huang** on passing his Ph.D. proposal exam. Rui's work continues the fast NMPC strategies developed by Victor and applies them to energy and power systems. Congratulations to **Rodrigo Lopez Negrete** on passing his Ph.D. qualifier exam. Rodrigo is also starting an internship at Pfizer on pharma process modeling and operation. Welcome back to **Brian Baumrucker** and **Anshul Agarwal**. Both were busy with summer internships at Air Products and Praxair, respectively.

Three new visitors will join Ignacio's group this fall: **Dr. Pedro Castro** from INETI, who will work on a project on batch scheduling with ABB, **Dr. Elvis Ahmetovic**, a Fulbright Scholar from Bosnia-Herzegovina, who will work in the area of process synthesis and biofuels, and **Elisabet Capon**, Ph.D. student from Dr. Puigjaner's group in Barcelona (UPC), who will work in supply chain optimization.

Congratulations to **Roger Rocha** for receiving the Outstanding Contributed Paper Award at the FOCAPO 2008 meeting that took place in Boston, June 29-July 2, 2008. The paper in question was:
"Petroleum Allocation at Petrobras: Mathematical Model and Solution Algorithm."

Congratulations to **Sebastian Terrazas** on passing his Ph.D. qualifier exam. Sebastian spent one month internship in Freeport, TX at Dow Chemical. Welcome back to **Fengqi You** and **Bora Tarhan**. Both spent their summer internships at Dow Chemical (Midland) and at ExxonMobil's Upstream Research Center in Houston.

Congratulations also to **Michael Wartmann**, who passed his Ph.D. qualifying exam. He also won travel scholarships to go to the American Control Conference, the PASI, and a CAST fellowship to go to the AIChE meeting. This Fall Michael is at the University of Delft where he is working on network modeling and control of oil and gas production systems in the North Sea.

Congratulations to **Eduardo (Wayo) Dozal** who defended his Ph.D. in April 2008 and **Yuan Xu** who defended his Ph.D. in May 2008.

CAPD e-News. We sent on April 23 our e-newsletter. We issue on a yearly basis two extensive newsletters with detailed descriptions of the projects in August and January, while the two others are brief e-Newsletters in April and October that contain short announcements as well as information that we think will be useful to the CAPD members, such as schedules of future professional meetings. We would appreciate receiving feedback or suggestions for improving the e-Newsletter.

2008 ANNUAL REVIEW MEETING

The Annual Review Meeting of CAPD took place on March 10-11, 2008. We had a record attendance of 39 participants from industry (ABB, Air Products, Aspen Technology, Bayer, BP, Cargill, Dow Chemical, Eastman Chemical Company, ExxonMobil, Kraft Foods, NETL, NOVA Chemicals, Paragon Decision Technology, PETROBRAS, PPG, Praxair, Pfizer, Simsci-Esscor/Invensys, Total). On the first day we had research overviews of the faculty, six excellent industrial presentations and a poster session. The dinner this year took place at Monterey Bay Fish Grotto Restaurant. On the second day, we had the presentations by final year students as well as a special session on Modeling Systems (see below). You can access an electronic version of the agenda, list of participants and slides presented at the 2008 CAPD Annual Review Meeting in: http://www.cheme.cmu.edu/internal/capd2008.pdf
Please take note that the next Annual Review Meeting will take place on **March 9-10, 2009.**

ENTERPRISE-WIDE OPTIMIZATION INTEREST GROUP

The project "Computational Models and Algorithms for Enterprise-wide Optimization of Process Industries," which is being partially funded by the Pennsylvania Infrastructure Technology Alliance (PITA), has continued with the participation of ABB, Air Products, BP, Dow Chemical, ExxonMobil, NOVA Chemicals and Total. The project involves a total of 7 Ph.D. students, and 5 faculty (CMU: Biegler,

Grossmann, Hooker; Lehigh: Snyder; UPitt: Schaeffer). A webpage describing this project, including seminar slides and meeting slides can be found in: http://egon.cheme.cmu.edu/ewocp/. The membership fee to join this group is $12,500 for members of the CAPD. Companies interested in participating in this research program should contact grossmann@cmu.edu.

Two companies have recently joined the EWO group: PPG and Praxair. The representative of PPG is Dr. Yu Jiao, and the one from Praxair is Dr. Jose Pinto. Dr. Ricardo Lima will work with PPG on the planning and scheduling of a multiproduct continuous plant, while the Ph.D. student Fengqi You will be working on a distribution problem by Praxair. The last EWO meeting took place on March 12, 2008, right after the Annual CAPD Meeting on March 10-11. We had a special session EWO on March 11 that was well received. The presentations were by Professor Sebastian Engell, University of Dortmund, Professor Tom Marlin, McMaster University, and Dr. Sridhar Tayur, SmartOps. The review of EWO projects took place on March 12 in which there was also a fruitful discussion about best practices in this area. The next EWO meeting will take place on **September 29-30, 2008**.

CAPD SHORT COURSE

We offered a new revamped short course on Optimization Modeling and Integrated Process Operations on June 12-18, 2008. Modules on Optimization Modeling were taught from Thursday through Saturday (June 12-15) focusing on modeling and algorithms with applications to process optimization, process synthesis and molecular design:
a) Nonlinear programming (Biegler, Thursday, June 12)
b) Mixed integer and disjunctive programming (Grossmann, Friday, June 13)
c) Global optimization and optimization under uncertainty (Sahinidis, Saturday, June 14)
Modules on Integrated Process Operations were taught from Monday through Wednesday (June 16-18-9) focusing on three major decision levels in plant and enterprise-wide optimization:
d) Mixed-integer models for planning and scheduling (Grossmann, Monday, June 16)
e) Process dynamics and control (Ydstie, Tuesday, June 17
f) Differential/algebraic models for real time optimization (Biegler, Wednesday, June 18)
The material in each module is independent and self-contained and can be taken in any combination. A detailed   description   of   the   topics   covered   in   the   course   is   given   in: http://capd.cheme.cmu.edu/shortcourse/shortcourse_details.htm
As an experiment we will offer the short course right after the CAPD and EWO meetings on **March 12-18, 2009**. For details see: http://capd.cheme.cmu.edu/shortcourse/index.html
 If you are interested in attending this course, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

PAN AMERICAN ADVANCED STUDY INSTITUTE ON EMERGING TRENDS IN PSE

Ignacio Grossmann organized with Frank Doyle, Jaime Cerda and Argimiro Secchi the Pan American Advanced Studies Institute (PASI) on *Emerging Trends in Process Systems Engineering* that took place on August 12-21, 2008, at Hotel Costa Galana, Mar del Plata, Argentina. The meeting was a great success and featured outstanding presentations. The workshop was aimed at advanced graduate and post-doctoral students, and emphasized the latest developments and research challenges in the emerging areas of *sustainability, energy, biological systems, multiscale systems, and enterprise-wide optimization*. This workshop was funded by NSF and the Department of Energy. We are grateful for the additional support that we received from GAMS Corporation, Cargill, Pfizer, PPG and Procter & Gamble. This allowed the participation of 50 Ph.D. students from the Americas (50% from U.S.). This PASI workshop was a follow-up to the successful PASI on Process Systems Engineering that took place on in Iguazú, Argentina, in 2005. The website for this meeting is: http://cepac.cheme.cmu.edu/pasi2008. Slides of the presentations and background material can be found in: http://cepac.cheme.cmu.edu/pasi2008/slides/index.html. This will become another virtual library as the one described below.

VIRTUAL LIBRARY ON PROCESS SYSTEMS ENGINEERING

The Pan American Study Institute on Process Systems Engineering that was organized by **Ignacio Grossmann** took place in Iguazu, Argentina on August 16-25, 2005. The workshop addressed four major areas: Optimization, Process and Product Design, Process and Supply Chain Operations, and Process Dynamics and Control. A major outcome of the PASI conference was the development of a virtual library on Process Systems Engineering covering the four areas. The library consists of the Powerpoint slides of the presentations, background articles, as well as exercises and MATLAB and GAMS computer files for various applications, and a practice exam with solutions. The virtual library can be found in, http://cepac.cheme.cmu.edu/pasilectures.htm

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that the CAPD newsletter is distributed in electronic form. We would appreciate receiving feedback from our member companies about our CAPD website, **http://capd.cheme.cmu.edu.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Work is under way to update and modify our website. Other websites of interest are Erik's http://mongol.cheme.cmu.edu/, Ignacio's http://egon.cheme.cmu.edu, Larry's http://dynopt.cheme.cmu.edu, and Nick's http://www.andrew.cmu.edu/user/ns1b/ Also, the department maintains the website of CEPAC (Chemical Engineering Pan American Collaboration), the organization that has been formed to promote collaboration between the US and Argentina, Brazil and Chile. You can find in http://cepac.cheme.cmu.edu/country.htm a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada, Mexico and Chile.

EXECUTIVE SUMMARY

Larry Biegler's Group

Since the last newsletter, a number of advances have been made in application of large-scale optimization, particularly for dynamic systems. The past few months have seen the following applications.

Dynamic optimization tools, ultimately for on-line use, have been applied that are centered on IPOPT, which continues to be developed at IBM. These have seen a number of applications ranging from detailed fuel cell models, advanced chromatographic separation, polymer reactors and processes, gas pipeline networks and nonlinear model predictive control. **Victor Zavala** has made strong advances in parameter and system identification for large-scale polymerization processes, and has developed a very efficient parallel computation approach. This is described in a preprint below. In addition, Victor has developed optimization formulations for Nonlinear Model Predictive Control (NMPC) and Moving Horizon Estimation (MHE) that exploit the simultaneous approach as well as recent NLP features in IPOPT. This has also been extended by **Rui Huang** to the control of air separation columns with detailed dynamic models. As a result, large dynamic optimization problems used for NMPC and moving horizon estimation (MHE) have *on-line computation costs reduced by two orders of magnitude!*

Related to this work is the development of specialized decomposition strategies within the IPOPT framework**. Brian Baumrucker** has developed interesting optimization formulations that incorporate complementarity constraints and allow a class of discrete decisions to be modeled within NLP problems. This approach is not restricted to particular NLP solvers and has been demonstrated on a variety of process applications. A preprint that describes this approach is listed below.

Finally, reduced order modeling strategies have been developed for large-scale PDE-constrained optimization. These are based on a snapshot-based decomposition and the isolation of principal components (i.e., eigenfunctions) that constitute the dominant elements of the solution space. Using these components as basis functions, one can create accurate reduced order models (ROMs) that are much

smaller and easier to solve than the original. This approach, originally due to Karhunen and Loeve has been used in two ways in this research group. In the first, we have applied ROM strategies to Fluent-based models to create reduced order optimization models for gasifiers and combustors. As described below and implemented by **Yi-dong Lang**, they make use of empirical input-output relationships described by neural network models. In the second approach, ROM strategies have been applied to pressure-swing adsorption (PSA) models. Here **Anshul Agrawal** has used these basis functions in a Galerkin framework to develop much more efficient models for gas adsorption. Both lead to much more efficient optimization strategies for dynamic systems.

Ignacio Grossmann's Group has been involved in the following developments:

In the area of optimization, **Juan Pablo Ruiz** has been applying to large process problems, a new solution approach for the global optimization of Bilinear Generalized Disjunctive Programming in which the lower bound is strengthened based on intersecting disjunctions following the recent Ph.D. thesis of Nick Sawaya. In collaboration with **Francois Margot, Pietro Belotti, Larry Biegler, and Nick Sahinidis**, the NSF project on Cyberinfrastucture has started with specifications for the case studies. Furthermore, the open source code *Couenne* for the global optimization of MINLP problems continues concentrating on branching rules and tightening of bounds for nonconvex NLP problems. **Aldo Vecchietti's** work on LOGMIP for disjunctive programming is now available in GAMS (http://www.gams.com/dd/docs/solvers/logmip.pdf).

Ravi Kamath, has developed novel mathematical models for multistream heat exchangers and for cryogenic distillation columns, as major modules for the optimization of IGCC plants. **Jose Caballero** has completed a manuscript using kirging models for the optimization of process flowsheets in order to handle implicit functions. **Ricardo Lima** completed the manuscript on optimization of crystallization of paraxylene, and undertook a project for PPG for cost estimation in batch manufacturing. **Gonzalo Guillen** completed two manuscripts for the bicriterion optimization of process networks in which the two criteria being optimized are economics (Net Present Value) and the Eco-indicator 99, a measure of sustainability, given uncertainties in the emission and damage data .

Bora Tarhan, has continued work in his Lagrangean branch and bound method for solving a multistage stochastic programming model for the design and planning of oil infrastructure planning under uncertainty. He has also explored the development of a scheme for updating MILP models in which the only change is in the coefficients of the objective function. **Sebastian Terrazas** has developed a unified framework for spatial and temporal decomposition schemes for multisite planning in continuous plants with changeovers. **Fengqi You** completed a new paper on stochastic inventory location-or supply chains. He also completed a paper on risk management for global supply chains with uncertain demands and freight charges, and has started a new EWO project with Praxair related to stochastic vehicle routing and tank-sizing. **Sylvain Mouret,** has developed an alternative MILP formulation for the crude oil scheduling problem, and tested symmetry breaking constraints through a constraint programming. **Abdul Attalas,** has been developing nonlinear aggregated CDU models, including methods for steam stripping, in order to go beyond the conventional fixed yield and swing cut models. **Roger Rocha**, a postdoctoral fellow from PETROBAS, has started to develop a clever disjunctive decomposition technique for petroleum large scale supply chain problems. **Pedro Castro** submitted a revision of the manuscript for the simultaneous batching and scheduling of batch processes with sequence dependent changeovers. **Antonio Flores-Tlacuahuac** from Mexico and **Sebastian Terrazas** produced a manuscript for simultaneous design, scheduling, and optimal control of a methyl-methacrylate continuous polymerization reactor. Finally, **Rosanna Franco** has completed the PC and web interfaces for the new NLP model the global optimization of integrated water systems by Ramkumar Karuppiah. See: http://newton.cheme.cmu.edu/interfaces/waternet/

Congratulations to Roger Rocha for receiving the Outstanding Contributed Paper Award at the FOCAPO 2008 meeting that took place in Boston, June 29-July 2, 2008. The paper in question was:
"Petroleum Allocation at Petrobras: Mathematical Model and Solution Algorithm."

Nick Sahinidis' Group

Nick's work falls into two main thrusts: (1) optimization theory, algorithms, and software and (2) applications of optimization to problems in biology, chemistry, engineering, and medicine. Research in optimization addresses the development of algorithms and software for: (a) global optimization of NLPs and MINLPs, (b) optimization of black-box models, and (c) linear programming. On the applications side, current activities address: (a) crystallographic computing, (b) protein structural alignment, (c) metabolic network modeling and design, and (d) design of compounds with desired properties.

Enabling Software From Nick Sahinidis' Group

Nick continues the development of BARON, primarily in collaboration with his former student **Mohit Tawarmalani**, who is currently an Associate Professor at Purdue's Krannert School of Management. In addition, students in Nick's group address theoretical and computational issues in global/local optimization. Their results are, from time to time, incorporated into BARON. The BARON software is currently available commercially under GAMS and AIMMS. In addition, a full blown version of the GAMS/BARON system is available entirely for free under the NEOS server for optimization. More information about BARON can be found at http://archimedes.cheme.cmu.edu/baron/baron.html.

Software for bioinformatics is also developed and maintained by Nick's group:
- CMOS: software implementing the Xie and Sahinidis algorithm for solving the contact map overlap problem for aligning the 3D structures of proteins
- R3: software implementing the Xie and Sahinidis residue-rotamer reduction for predicting the structure of protein side chains
- SBH: software implanting the Chang and Sahinidis algorithm for finding all near-optimal solutions of the combinatorial problem in DNA sequencing by hybridization

Nick's web site at http://archimedes.cheme.cmu.edu/group/biosoftware.html provides these codes as on-line solvers.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: Victor M. Zavala (Ph.D. started Fall, 2004)
Visitor: Kexin Wang, Zhejiang University

As a result of several generations of Ph.D. students, we now have a number of very efficient NLP algorithms including rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. As described above, the most recent incarnation is IPOPT, with continuing development by Andreas Wächter. This code has become a core algorithm for many of the research projects described below. In his Ph.D. thesis, Carl Laird has applied IPOPT and the AMPL interface to develop a novel source detection strategy for municipal water networks as an important application for barrier methods. This optimization problem is developed to detect attacks on networks and to determine optimal control and remediation strategies. By exploiting the structure of these networks, discretized problems that represent actual municipal networks with up to 300,000 variables could be solved in only a few CPU seconds. More recently, this approach has been extended, by using an MIQP strategy, to a more robust one that promotes unique solutions. Using an efficient pre-processing step, small subproblems can be derived and attack scenarios can be identified more precisely and efficiently. This approach is described in the preprint below.

Finally, the new version of IPOPT continues to updated and maintained. Designed in C++, this code is object oriented and flexible to deal with a wide variety of linear solvers, new barrier algorithms, and a variety of globalization strategies and decomposition approaches. Moreover, as noted above, the new code

provides a much easier interface to modeling environments. Carl has expanded the IPOPT code to accommodate in the following ways:

- Multi-scenario problems are essential to deal with process optimization under uncertainty and have a structure that can be decomposed through Schur complements and can be completely parallelized on distributed memory machines. Carl has obtained some excellent results with this decomposition that validate these properties.
- More recently, Victor has demonstrated this approach on a large-scale parameter estimation problem, executed on parallel processors and show essentially perfect speedups with this approach. A preprint that describes this approach is listed below.
- The structure of IPOPT has been expanded to deal with NLP sensitivity. This approach very quickly provides an estimate of the solution of a perturbed NLP problem. As a result, it is very useful for quickly solving a sequence of problems that change only slightly from the previous one. This is applied below to develop a very fast strategy for Nonlinear Model Predictive Control (NMPC).
- The reduced-space, FORTRAN version of the IPOPT code is also being extended by **Kexin Wang** to included recent developments in the IPOPT project. This will also allow the incorporation of recent penalty-based barrier methods developed by Chen and Goldfarb to be adapted to the reduced space approach. In addition, Kexin has recently implemented and tested a new restoration phase for the reduced space approach. This approach deals with linearly dependent constraint gradients along with rapid detection of infeasible constraints.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: Brian Baumrucker (Ph.D. started Fall, 2004)
Gaurav Bansal (MS started Fall, 2006)

MPECs represent an exciting new field in mathematical programming. While applications of MPECs have long been recognized in game theory, transportation planning, economics and engineering design, little work has been done in developing efficient algorithms for their solution In process engineering, these problems stem from bilevel and multilevel optimization problems as well as optimization of hybrid (discrete and continuous) systems. Included in this class are optimization problems with phase equilibrium constraints, as in equilibrium stage processes.

The MPEC problem is essentially a nonlinear programming problem augmented by complementarity conditions. The addition of these conditions leads to a violation of convergence assumptions for most nonlinear programming algorithms (e.g., linear independence of the constraint gradients) and can cause these algorithms to fail. On the other hand, the barrier method described above has a straightforward extension to these problems. As a result, complementarity constraints can be incorporated with little additional cost in the algorithm. In fact, all of the features that contribute to the efficient performance of IPOPT can be invoked directly for the solution of the MPEC problems. The resulting algorithm based on IPOPT has been developed further and refined for a number of challenging dynamic optimization applications in process engineering. Our work in this area includes the following:

This project builds on the Ph.D. work of Arvind Raghunathan. In his research, he has incorporated the MPEC formulation into the IPOPT code, now called IPOPT-C, along with algorithmic modifications to treat the complementarity constraints more efficiently. This code has been interfaced to the AMPL modeling system and has been tested on a set of library MPEC problems. Our results show that this implementation compares well against competing barrier algorithms such as LOQO. Arvind tested this approach on a number of process optimization problems with phase equilibrium constraints. These include distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages, dynamic systems with switching conditions, such as overflows and phase disappearance in distillation columns and metabolic network systems.

For the latter, we have considered parameter estimation problems for dynamic fermentation systems for wine production. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies. Related work initiated by **Juan Arrieta** deals with modeling and optimization of dynamic biological systems that are based on cellular models. Such systems are large-scale extensions of MPECs, which arise from the metabolic flux models represented as linear programs. In particular, it is easy to show that these MPEC models capture all of the solutions of LP models and provide a fully continuous problem formulation. Moreover, they have interesting modeling features since state dependent constraint functions with discontinuities also need to be treated through MPEC formulations. **Gaurav Bansal,** who recently completed his MS and joined Bayer Corporation, has expanded the capabilities of these formulations along with the consideration of larger, extended models for yeast fermentation. In his MS thesis, he demonstrated the use of the penalty formulation for MPECs on these models.

In extending MPEC optimization formulations, **Brian Baumrucker** is currently considering the development of good MPEC formulations that model discrete decisions. He has explored these with the ROMeo real-time optimization package along with formulations for complementarity conditions within real-time optimization models. In particular, he has shown that penalty-based NLP formulations have worked very well on these models. Moreover, with these formulations, one is able to decouple problem-specific optimization algorithms from the optimization model and rely on general purpose optimization solvers. In addition to the ROMeo comparison described above, he has investigated complementarity formulations in distillation columns with mass transfer limitations as well as the operation and scheduling of dynamic pipeline models. Working with colleagues from Air Products, Brian has shown that complementarity formulations embedded within a dynamic optimization formulation. This allows the optimal exploitation of inventory in pipelines in order to reduce energy and other operating costs, while still meeting customer demands.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Researchers: **Victor Zavala (Ph.D. completed August, 2008)**
Rui Huang (Ph.D. started Fall, 2006)
Weijie Lin (Ph.D. started Fall, 2006)
Rodrigo Lopez Negrete de la Fuentes (Ph.D. started Fall, 2007)
Yi-dong Lang (Jiansu Research Institute, Nanjing, China)

The topic on simultaneous solution and optimization strategies for large-scale, dynamic optimization problems incorporates a number of projects. In the past, we have applied this approach to optimization problems for batch reactors, process dynamics and tray-by-tray batch distillation and large-scale dynamic flowsheeting models. Moreover, we have tackled dynamic examples successfully with this approach that cause any sequential dynamic optimization method to fail. Two fundamental studies on simultaneous solution approaches, with Shiva Kameswaran, are described in the reprints below. The first, published in *SIAM J. Scientific Computing*, deals with the advantages of this approach for high index algebraic constraints, for which adjoint profiles do not exist. The second, published in *Comp. Optimization and Applications*, provides a rigorous analysis on the convergence of Radau collocation approaches to the infinite dimensional solution of the optimal control problem. This paper classifies the problem types considered, describes a number of advantages of the simultaneous collocation method and provides convergence rates for collocation schemes.

In addition, the following research projects are currently being addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization, one based on reduced space and one on full space. First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called ***DynoPC***. Written for Windows with a Visual Basic user interface and with heavy integration of graphical, simulation and automatic

differentiation tools, this software package incorporates our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from http://coin-or.org   Current developments with *DynoPC* include ESO interfaces that are compliant with recently developed CAPE-Open protocols. This leads to an interface compatible with a number of existing process models and modeling environments.

Second, we have been using IPOPT in a full space framework linked to the AMPL modeling environment. As detailed in many of the studies listed below, this framework has been extremely powerful and flexible in solving a wide variety of problems. A MATLAB framework has been coupled to the AMPL modeling language and domain specific prototypes have already been developed and work very well. In addition, Johan Akesson, a previous visitor who recently received his Ph.D. from Lund University, has developed a Modellica framework that works with IPOPT and AMPL. In a recent study, he was able to optimize an open-plate reactor with over 100,000 variables in about an hour of CPU time. More recent studies are listed below as reprints in which structured properties of the optimization problem (such as *block bordered diagonal* and *almost block diagonal*) are exploited in order to solve much larger problems.

Large-scale Parameter Estimation for Polymerization Processes

In a project funded by ExxonMobil Chemicals, **Victor Zavala** has developed multi-stage dynamic optimization problems for grade transition and nonstandard operations. For this, he has developed a detailed reactor model of a polyolefin reactor, which includes a complete kinetic description that is used for parameter estimation using actual process data. Using AMPL and IPOPT, Victor has extended this model to multiple data sets as well as EVM problems (where errors in both inputs and outputs are considered). Applying this approach to a large number of data sets, Victor was able to estimate kinetic parameters quite well; the scatter of the data was reduced by an order of magnitude, compared to previously fitted models. Moreover, using the NLP sensitivity approach described above, Victor has recently shown that the covariance matrix from a maximum likelihood formulation can be extracted easily from IPOPT using a few additional back-solves of the KKT matrix. This allows statistical inference to be added efficiently to parameter estimation studies. This has recently led to a novel moving horizon estimation scheme which is described in the preprint below.

Weijie Lin is working on process model development for an advanced polymer product. The approach is similar to the moment models developed by Victor, but with more complex features dealing with the polymer structure. Weijie's preliminary work has shown the importance of parameter estimation for this large-scale model in order to demonstrate structurally dependent features (e.g., gel effect, cage effect, glass effect) on the polymer reactions. This also allows her to develop MW distributions of the complex polymer network. So far, she has developed novel particular models that deal with polymer kinetics and growth. She has compared this model with industrial data and completed a detailed parameter estimation study. As a result, she has been able to validate the model and also suggest future directions for the experimental program as well. With the successful completion of this work, Weijie has started to investigate optimal control strategies that improve the product quality and reduce production time. Preliminary results indicate significant performance gains can be obtained with quite different, novel operating strategies.

Nonlinear Model Predictive Control Strategies

In less than two decades, Nonlinear Model Predictive Control (NMPC) has evolved from a conceptual framework to an attractive, general approach for the control of constrained nonlinear processes. These are based on the on-line solution of optimization problems for control. One such approach, which we conducted with researches in Switzerland, is listed as a reprint below. The advances in NMPC were realized both through better understanding of stability and robustness properties as well as improved algorithms for dynamic optimization. The above dynamic optimization algorithms have been applied extensively in Nonlinear Model Predictive Control (NMPC). This strategy is also being extended to large-scale models for polymerization processes.

In addition, we recently adapted the *real-time iteration* approach developed in the context of multiple shooting (Diehl et al. (2006); Bock et al. (2006)) to a collocation-based approach with a full space nonlinear programming solver. Over the past year, we show that straightforward sensitivity calculations from the KKT system also lead to a real-time iteration strategy, with both shifted and non-shifted variants. These are described in a reprint below. This leads to an NMPC strategy called the Advanced Step NMPC Controller. Demonstrated on a large-scale polymer process, the Advanced Step Controller leads to on-line calculation effort that is reduced by over two orders of magnitude. As described in a paper soon to appear in *Automatica*, we have been developed a general Lyapunov-type stability analysis for this approach that demonstrates nominal stability, input to state stability and robustness margins to noise and model mismatch. This recent development has been extended to moving horizon estimation (MHE) for parameter and state identification and yields the same dramatic improvements in performance. This result was recently presented in a keynote paper at the DyCOPS meeting and is listed as a reprint below. A further reprint is also listed, where Victor shows the potential of combining both fast NMPC and MHE steps in one to yield controllers that are tolerant to noisy data and drifting model parameters. This paper will be a featured presentation at the upcoming NMPC '08 Conference in Pavia, Italy.

Rui Huang, has recently adapted this work to NMPC distillation control and advanced power plant systems. His preliminary work has demonstrated that the Advanced Step NMPC also reduces on-line calculation time by about two orders of magnitude. The resulting application deals with a detailed air separation (double) column with about 1500 DAEs and an NLP with over 100,000 variables and equations. Although the problem can be solved in less than 4 CPU minutes, the on-line computation is still very much faster. Rui's results indicate that the NMPC controller requires only a single second of CPU time. A reprint (soon to appear in *J. Process Control)* is listed below and provides full details of this approach.

Finally, **Rodrigo Lopez Negrete** has recently joined the group and is extending this approach to stochastic processes with uncertainties in states and outputs. Also, he is adapting recently developed Unscented Kalman Filter (UKF) methods, which deal with non-normal noise structures, to the MHE formulation. In recent tests, Rodrigo has shown that this strategy has superior performance to Kalman Filter approaches and previous MHE strategies.

Large-Scale Optimization for Fuel Cell Models

Researchers: Parag Jain (Ph.D. started Fall, 2005, joint with Prof. M. S. Jhon)

In his thesis project, Cong Xu initiated the investigation of optimization problems arising in fuel cell applications, including Direct Methanol Fuel Cells (DMFCs) and Hydrogen PEM fuel cells. In particular, he has extended simple DAE models for fuel cells to consider optimal flow patterns and minimization of contamination effects due to membrane crossover, and he has extended these models to consider sensitivity and optimization calculations. In particular for DMFCs, we have compared and critically assessed several literature models and have explored the crossover phenomenon. By applying our dynamic simulation and optimization tools, they were able to develop dynamic feeding strategies for these systems that greatly reduce contamination due to methanol crossover. The results show that the optimal design of DMFCs can be achieved without pulsed operation. Here crossover is significantly reduced and the power density is correspondingly increased. The efficiency of these processes can also be improved through flowsheet optimization strategies as well as heat integration of the process units. This approach is based on conventional flowsheet optimization schemes within Aspen/Plus along with simultaneous optimization and heat integration strategies. The application to fuel cell based processes leads to interesting trade-offs between the fuel cell, the rest of the flowsheet and the heat recovery system.

Dynamic optimization has also been applied by Shiva Kameswaran to develop ramping strategies for fuel cell power plants. In a project funded by Fuel Cell Energy, Inc. and DOE, Shiva has demonstrated significant improvements in maintaining power levels with more energy efficient operation. Using AMPL and IPOPT, he has incorporated detailed models of the entire power plant and has demonstrated this approach both for parameter estimation and optimal control. Currently, **Parag Jain** has extended previous modeling and optimization work for Hydrogen PEM Fuel Cells. He has applied a comprehensive two-dimensional computational model of a PEM fuel cell that accounts for major transport processes including

membrane electrode assembly (MEA) and gas distribution channels. Additionally a water transport model in the membrane has been developed and incorporated into the full PEM fuel cell model. Using AMPL and IPOPT, Parag is using this model to develop a detailed optimization case study. The results of this work are listed in a reprint below. More recently, Parag has extended this work to assess the role of platinum distribution in the catalyst layer. As discussed in the preprint below, this approach leads to an exponentially damped Pt profile in the catalyst layer that leads to significantly higher power densities for the PEM Fuel Cell. Moreover, these results lead to novel optimization-based strategies for improvements in membrane design coupled with catalyst loading.

Dynamic Optimization for Semi-Closed Process Models
Student: **Sree Ram Raju Vetukuri (Ph.D. started Fall, 2006)**
Collaborator: **Prof. Andrea Walther (Technical University of Dresden)**

This project explores the application of recent developments in automatic differentiation and nonlinear programming to semi-closed process models, including systems solved with DAE integrators. This sequential optimization approach for dynamic systems has been the competing strategy to the simultaneous optimization approach adopted in our group. It has advantages for problems where error control is especially important, where many time steps are needed and where these need to be adjusted frequently during the integration. Recent years have seen the development of efficient sensitivity strategies to obtain accurate first and even second derivatives for use in dynamic optimization algorithms. However, this approach becomes inefficient when there are many degrees of freedom. For instance, in the optimization of Pressure Swing Adsorption units, Ling Jiang developed an efficient sequential dynamic optimization approach. However, when several hundred inputs were considered in the model, the optimization required hundreds of CPU hours.

This bottleneck has recently been addressed by a recent SQP-type algorithm that uses exact right hand sides of the KKT equations, along with Jacobian-vector and Hessian-vector products, but computes only inexact Jacobians. Using leading edge technology in automatic differentiation, these quantities can be computed orders of magnitude faster than with the standard sequential approach. Profs. Andreas Griewank and Andrea Walther have recently developed a globally convergent SQP that uses inexact Jacobians, called TR1. Based on a composite trust region strategy, this approach has recently been applied to periodic adsorption processes as well. **Sreeram Vetukuri** has extended this approach using ADOL-C for automatic differentiation and CVODES for sensitivity calculations of first and second derivatives, and interfacing to TR1. Preliminary results on a small SMB system show the potential of this algorithm for reducing CPU time. More recently, he has extended this approach to Pressure Swing Adsorption (PSA) systems that have more complex dynamic behavior, with a broader spectrum of time scales, and more complex mass transfer and equilibrium behavior. The resulting approach has led to a more comprehensive and efficient approach to PSA optimization. This work will be presented at the upcoming AIChE meeting and a preprint will be listed in the next newsletter.

Reduced Order Models for PDE-based Units in Power Plant Flowsheets
Researcher: **Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Students: **Anshul Agarwal (Ph.D. started Fall, 2005)**
            Adam Malacina (MS completed May, 2008)

Process simulation has become an essential capability that spans most tasks in process engineering, design and analysis. Simulation programs such as Aspen Plus, Pro/II and HYSYS are integrated into core engineering design activities. However, due to computational limitations, current process simulators usually deal with lumped parameter models that often do not capture detailed spatial characteristics of process units, including fluid flow and transport processes. As a result, they can suffer accuracy limitations and the loss of predictive capability. To overcome this difficulty, we are working with NETL on the Advanced Process Engineering Co-Simulation (APECS) project. Within this framework, process flowsheeting models (in Aspen Plus) have been successfully combined with computational fluid dynamics (CFD) models (using Fluent) to model multiphase systems, such as gasifiers and turbines within power plants. Current efforts are also focused on the inclusion of other distributed parameter custom models. In particular, an important, and challenging, application for this activity is the FutureGen Cycle, a 275 MW

coal-fired power plant that includes hydrogen generation and CO2 recovery, and requires multi-phase, spatially distributed models within its simulation environment.

To extend these NETL activities, we are developing and applying integrated optimization strategies that provide powerful tools for model development and process improvement. So far, these optimization problems are small-scale and efficient, and robust optimization algorithms are available that can be implemented easily. These features have led to the relatively easy and widespread adoption of optimization strategies. On the other hand, optimization strategies for CFD and distributed parameter models have seen far less development and this currently represents an important and challenging research activity. For APECS, which incorporates these models, we believe that optimization strategies will perform a key role in the development of advanced energy processes, such as the FutureGen Cycle. To provide a vehicle for the research tasks in this project, we consider the model components of the FutureGen Cycle flowsheet. This process includes a number of unit operations for coal gasification and byproduct (e.g., ash/slag and sulfur) separation; multiphase CFD models are needed for this purpose. Yi-dong Lang has been working with colleagues at Fluent Corp. to develop reduced order CFD models based on Proper Orthogonal Decomposition (POD) and Principal Components Analysis (PCA). This approach allows for a tremendous reduction in computing effort for the process flowsheet. Yi-dong has considered a PCA based approach coupled with an efficient experimental design approach along with a neural network solver to determine an input output model. Using an NETL-based Fluent combustor model, he has developed accurate reduced order models (ROMs) that capture the behavior of the Fluent model over a wide input range, but with require about two orders of magnitude less execution time. As a result, these models are quite suitable to incorporate within FutureGen process flowsheet. **Adam Malacina** recently completed his MS thesis and has joined UOP. In his MS thesis he applied and extended Yi-dong's approach to a FutureGen gasifier model, also developed in Fluent. While the gasifier model was somewhat more involved than the combustor model, the PCA-based approach worked very well and led to an accurate reduced order model for further process optimization.

Further downstream of the gasifier in the FutureGen process, the byproduct gases CO2 and hydrogen are separated and CO2 is sequestered. These separations can be performed effectively by pressure swing adsorption (PSA) units, which operate dynamically and require the calculation (and subsequent optimization) of cyclic steady state behavior. Such models were considered in the PhD thesis of Ling Jiang. While her optimization approach was very successful for large-scale PSA units, it still required many hours of CPU time, and therefore requires custom reduced order models (ROMs). Over the past year, **Anshul Agarwal** has been developing reduced order models for these units as well using a novel space-time discretization to develop the ROM using a POD-based approach. A key advantage of this approach is that very small models are developed that can be discretized in time (using collocation on finite elements) and solved with AMPL and IPOPT. Preliminary results by Anshul show that this strategy can lead to very efficient optimization strategies. This approach will be published shortly in *I&EC Research.*

Finally, both Anshul and Sreeram have developed a novel superstructure for the evaluation of CO2 capture strategies using PSA. Following on recent work by Ritter, Webley and their coworkers, this approach captures a number of different PSA steps (e.g., pressurization/depressurization, adsorption/desorption, pressure equalization, light and heavy product recycle) through the formulation of an optimal control problem. Preliminary results indicate that the superstructure is rich enough to predict both high purity and high recovery of captured CO2. It is therefore quite useful in predicting the suitability of different sorbents and operating strategies for PSA.

Ignacio Grossmann's Group

Cyberinfrastructure for MINLP Optimization

New developments: **Outline of library MINLP problems; Open source code *Couenne***

Student: **Juan Pablo Ruiz [started Jan 2007]**
Post-doctoral fellow: **Pietro Belotti (Tepper)**

Collaborators: Larry Biegler, Nick Sahinidis, Francois Margot, Gerard Cornjuelos (Tepper)

We have been funded by NSF on a new project that has as objectives to create a cyberinfrastructure environment for virtual collaboration for developing and collecting tools for MINLP, including a library of challenging MINLP test problems. In addition the objectives are to develop basic algorithms, formulations for predicting tight lower bounds, and open-source software for solving large-scale nonconvex MINLP problems (e.g. Couenne). We also aim to test the software with challenging problems arising in real-world applications, mostly in engineering but also in biology and finance

One of the main components of the website will be a collection of MINLP problems in which instead of simply providing input files in GAMS, AMPL, AIMMS or similar, we will develop a library of problems where we present them first in their qualitative form by describing its problem statement, presenting one or several formulations with detailed derivations, data for one or several instances, and results for one or several solvers. For each instance input files will be provided. We are currently at the stage of developing the specifications for these problems as well as the structure of the website that will feature a wiki for each problem in order to promote discussion and comparisons. We should have the webpage and an initial collection of problems ready by the end of October.

In this project Pietro Belotti is also developing the *Couenne* an open-source code for solving nonconvex NLP and MINLP problems. The goal is to develop both approximate as well as rigorous methods that rely on the use of convex envelopes and bound tightening strategies. The rigorous method relies on a spatial branch-and-bound method for bilinear, linear fractional and concave separable functions. Parametric linear convex envelopes are obtained by breaking a nonlinear expression into compositions of simple operators for which convex linearizations are known. By introducing additional variables, a linear convex envelope of the original expression can be obtained. This polyhedral envelope is a function of the upper and lower bounds on the variables and it becomes a tighter approximation when upper and lower bounds on the variables are moved closer. This can be exploited in a branch-and-cut algorithm by branching on continuous variables, i.e. splitting the domain of its possible values. These parametric convex envelopes can also be used to generate an infinite number of valid linear cuts, raising interesting questions regarding cut selection and cut strategy when integrated in a branch-and-cut framework. Pietro has written the code CouenneSolverInterface that allows the implementation of various bound tightening techniques, and branching strategies. Pietro will be moving to Lehigh as a Visiting Assistant Professor, but will continue to collaborate with us.

Algorithms for Nonlinear Disjunctive Programming

New Developments: Application to process problems; LOGMIP in GAMS22.8

Student: Juan Pablo Ruiz [started Jan 2007]
Research collaborator: Aldo Vecchietti [Researcher at INGAR]

Juan Ruiz

The project of Juan is concerned with the global optimization of non convex Generalized Disjunctive Programs. These problems arise, for instance, in the design of pooling problems, in the synthesis of integrated water treatment networks, or generally in the synthesis of process networks with multicomponent flows. Juan's work has, as a major objective to improve the computational efficiency of disjunctive spatial branch and bound methods by combining the relaxation strategies proposed by Tawarmalani & Sahinidis (2002) for nonconvex MINLPs with the results in the work of Sawaya & Grossmann (2007), closely related to the work of Balas (1985), to obtain tighter relaxations for Linear GDPs.

The basic approach consists of first relaxing the non convex terms in the GDP using suitable convex under/over linear estimators and the convex nonlinear terms with suitable linear outer approximators

Tawarmalani & Sahinidis (2002) and introducing them as part as the disjunctive set. Since the corresponding relaxation leads to a linear GDP problem, the next step then consists of performing basic steps which involve intersecting disjunctions in order to obtain tighter relaxations as outlined in Balas' theory. Of course there are many options that are possible on how to perform the intersections.

To address this issue Juan has made use of a Theorem by Balas that states general conditions under which basic steps are or are not necessary. The conditions in this theorem are difficult to verify in general since it may require knowing if new extreme points are generated when applying the basic steps. However, insight can be obtained by exploiting the particular structure of the formulations. Based on this, and considering structures commonly found in process models, Juan has developed a set of sufficient conditions under which basic steps are not necessary. Using these propositions as a basis as well as other properties, he has developed a procedure that relies on the following rules: 1. Basic steps are applied between disjunctions with at least one variable in common (The more variables in common the more tightening can be expected). 2. If non convex terms are outside the disjunctions, apply basic steps by introducing them in the disjunctions (if nonconvex terms are inside disjunctions less tightening can be expected); The solution method then consists in first applying this reformulation procedure, leading to a tight relaxation, then applying the bound contraction method by Juan Zamora, and finally applying a branch and bound procedure similar to the one that Sangbum Lee had developed in which branching is performed first on the discrete variables.

Two particular cases were studied, namely, Bilinear GDP and Concave. Following the method described above, Juan has applied his reformulation to several process systems problems, such as the design of wastewater treatment networks, pooling networks, distillation sequences with pooling integration, HEN with discontinuous Investment Cost and retrofit of HEN. In these cases the non convexities came either by the bilinear terms in mass balances around splitters and energy balance around heat exchangers or by the concave terms in cost functions which consider economy of scale. In all cases a clear tightening effect compared to the traditional method proposed by Lee and Grossmann 2003 was observed. Future lines of research consider the implementation of a hybrid approach of the bound contraction method with the branch and bound procedure where the model used in the latter is not the same as the model used in former. First results of this approach have shown important improvements in the efficiency of the method.

Aldo Vecchietti: LOGMIP and DICOPT

Aldo and his students at INGAR in Argentina have developed the LogMIP code, an extension of the GAMS modeling language for posing logic/disjunctive problems. The syntax developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. The definition of disjunctions over sets and subsets can also be specified. As for the propositional logic, the special constructs ATLEAST, ATMOST, EXACTLY are defined to specify that the sum over a subset of variables with a given cardinality is at least, at most or equal to one. Also, LogMIP can now accept logic propositions in symbolic form without the need of translating them into linear inequalities.

For solving linear disjunctive/hybrid problems LOGMIP can automatically generate the convex hull relaxation and big-M transformation for linear problems. Aldo has also automated the logic-based OA algorithm by Metin Turkay, which is suitable for nonlinear GDP process network problems. GAMS is releasing LOGMIP in the new version 22.8 For the corresponding manual see: http://www.gams.com/dd/docs/solvers/logmip.pdf. Plans are underway to implement the big-M and convex hull transformations with the help of GAMS in LOGMIP.

Optimal Synthesis of Integrated Gasification Combined Cycle (IGCC) Systems

New developments: **Models for air separation unit, multistream exchanger**

Student: **Ravi Kamath [Ph.D. started Jan 2007]**

Ravi successfully passed his Ph.D. qualifying exam. This is a new project within the newly established Institute of Energy Solutions that is being funded through NETL. The objective is to develop a

comprehensive synthesis model for IGCC plants, with the possibility of polygeneration and CO_2 sequestration. Integrated Gasification Combined Cycle (IGCC) technology for future power plants has attracted great interest because of its capacity to not only achieve a higher thermal efficiency but also capture CO_2 more economically than a conventional coal-fired plant. However, IGCC technology has higher capital costs than coal-fired plants and is economically viable only if operated with CO_2 capture. Ravi's project will aim at evaluating the techno-economic performance of an IGCC plant. We assume that we are given a type (rank, quality, composition, physical state) of coal, net output power, location of site, ambient conditions for utilities like air and water and other requirements like co-production of hydrogen or chemicals and extent of carbon capture. The objective is to determine the optimal structural configuration and operating parameters of the IGCC plant that minimize the investment and operating cost, while meeting the constraints for environmental emissions. An important related decision will be the minimum amount of CO_2 to be captured.

As a first step, Ravi developed a comprehensive superstructure that includes potential alternative technologies. The goal is to determine the optimal configuration and operating parameters for the IGCC flowsheet by formulating a mixed-integer nonlinear programming (MINLP) problem. Because of the large number of alternatives, we intend to apply the methodology developed by Mark Daichendt that involves optimizing the entire flowsheet at different levels of complexity using a combination of aggregated and detailed models. As indicated in the last newsletter, Ravi developed simplified models for coal gasification and for the utility section. For coal gasification he developed a model based on Gibbs energy minimization that can be modified to match the performance of real gasifiers. This is done by adding equilibrium reactions as constraints, or additional specifications to match outlet compositions. He has obtained very good results for the Shell, GE and ConocoPhilips entrained gasifiers. The prediction of the main eight species is in close agreement with published data. Ravi also developed an MINLP model for combined cycles that extends the MINLP model by Bruno. The basic idea consists of postulating a superstructure for the specified power and heating demands. The superstructure is modeled as an MINLP in which pressures and temperatures of steam, enthalpies, and turbine efficiencies are treated with nonlinear models. For an example with an electricity demand of 500 MW, 2 mechanical power demands, and steam demands at high, medium and low pressure, Ravi was able to obtain good results from the MINLP model that involved 44 0-1 variables, 1275 continuous variables and 1309 constraints.

In the last few months Ravi has concentrated on the development of the flowsheet and optimization model for the Air Separation Unit (ASU), which supplies high pressure oxygen (> 95% purity) to the gasifier and medium pressure nitrogen to the gas turbine. A real industrial flowsheet for air separation involves 2 complex columns which are thermally integrated in such a way that heat load of the condenser of high pressure (HP) column matches that of the reboiler of the low pressure column. Also included in the flowsheet are multiple feeds and side-draws that are heat-integrated using two multi-stream heat exchangers. The step-wise construction of the flowsheet can help in understanding why such a complicated heat integration involving multiple streams is preferred over a simple configuration by evaluating material and energy costs at each step in the flowsheet construction. Since writing rigorous models from the start could lead to convergence problems, Ravi tried to focus on the use of simplified or short-cut type models for the complex distillation columns. Ravi extended the Edmister model for counter-current cascades by replacing some of the poor approximations by more realistic constraints based on physical insight. The result of this work is an aggregate model for a counter-current cascade of trays in a distillation column whose performance closely resembles that of rigorous models of Aspen Plus. Just like the rigorous tray-by-tray model, our proposed model does not require knowledge about key components or about whether it behaves as an absorber or a stripper. Ravi has demonstrated the efficacy of this model using both simulation and optimization case studies. Test problems involve distillation of binary and ternary systems with ideal or mildly non-ideal thermodynamics. In the case of simulation case studies, the outlet conditions at the top and bottom are analyzed for a given set of input parameters (e.g. number of trays, column pressure, reflux ratio etc.). In the case of optimization case studies, the objective is to determine the optimal feed locations and/or optimal number of trays that minimize capital and/or energy costs while meeting the specified purity requirements. Results for the simulation case studies show that the outlet conditions predicted by the aggregate model are in close agreement with that of the rigorous model. For the optimization case studies, a rounding heuristic can be used i.e. the number of stages in the cascades can be relaxed as continuous variables and their optimal value can then be rounded to the nearest integer. In most

cases, the integer solution obtained by this rounding heuristic was found to be the same as the integer solution of the MINLP model. Thus, use of integer variables can be eliminated for the aggregate model and its solution provides a good approximation to that of rigorous model (often missing by only one or two trays).

Ravi then started to develop models for the multi-stream heat exchangers (MHEX). It is to be noted that modeling MHEX is not trivial because of two reasons: a) Matches between hot and cold streams are not known *a priori* b) Since the matches are not known; it is not clear how to apply the criterion of minimum temperature driving force. Moreover, MHEX have complex hardware designs and the streams involved typically undergo phase change during heat transfer. There are hardly any simulation or optimization based process models for MHEX available in the open literature which take care of issues like violation of minimum temperature driving force or temperature cross-overs. Optimization of flowsheets containing one or more MHEXs can be regarded as a case of simultaneous optimization and heat integration where the inlet and outlet streams conditions of MHEXs are optimized simultaneously along with the rest of the process variables in order to minimize overall cost while satisfying the constraints imposed by external process as well as feasible heat transfer constraints inherent for MHEXs.

Ravi has developed a general nonlinear equation-oriented model for MHEX which is based on pinch technology for heat integration. A special feature of the model is its capability to detect phase changes and accordingly calculate enthalpies. Candidate streams which are capable of phase changes are split into three substreams corresponding to superheated (SUP), two phase (2P) and subcooled (SUB) regions. This splitting is based on dew point and bubble point temperatures of the stream that may change during the course of the optimization as pressure and composition of the stream are treated as process variables and can be optimized. From the point of view of heat integration, each of the above substreams can be treated as an independent stream with an associated heat load and inlet and outlet temperatures. The inlet and outlet temperatures of substreams are assigned appropriate values using a disjunctive representation involving Boolean variables (Raman and Grossmann, 1994) where the Boolean variables are associated with the phase of parent stream at the inlet and outlet conditions. The disjunctions can be formulated either as a discrete-continuous model involving binary variables (Lee and Grossmann, 2000) or as a continuous model by solving an inner minimization problem with complementarity constraints (Raghunathan, 2004). Also, when a candidate stream does not change its phase, the inlet and outlet temperatures of irrelevant substreams are manipulated in such a way that the associated heat loads are set to zero. It is to be noted that this representation assumes that the enthalpy of the streams can be approximated as a piecewise linear function of temperature in each of three regions. If necessary, the two phase region in particular can be split further into more segments to improve this approximation. Ravi has demonstrated the capability of this model for MHEX using the PRICO (Poly Refrigerant Integrated Cycle Operations) process for LNG production (Lee et al., 2002). Although the PRICO process is a relatively simple process involving a single mixed refrigerant circulating in a simple cycle, it incorporates most of the components present in more complex LNG liquefaction processes. The proposed model is used within a mathematical programming formulation to determine the optimal operating conditions and composition of mixed refrigerant that minimizes the shaft work required for vapor compression.

Using these equation-oriented models, Ravi is currently implementing the superstructure for the ASU flowsheet in GAMS which can be solved as a simulation problem or also as an optimization problem. Then, he plans to focus on other sections of the IGCC plant such as acid gas cleaning and CO_2 absorption.

MINLP Flowsheet Optimization with Process Simulators

New developments: **Acceptance of paper for flowsheet optimization using kirging model**

Collaborators: Jose Caballero [Associate Prof., Univ. Alicante]

While most of the work with Jose Caballero has concentrated on thermally integrated separation sequences, one additional piece of work has been the incorporation of process simulators for MINLP optimization in process flowsheets. Beyond the work reported in the last newsletter for solving Process Synthesis problems

with GDP and MINLP models, Jose has concentrated his efforts in the NLP optimization of flowsheets implicit models.

Jose's work has addressed the rigorous optimization of nonlinear programming problems in which the objective function and (or) some constraints are represented by noisy implicit black box functions such as in process simulators in which the derivatives are not available and some units operations introduce noise preventing the calculation of accurate derivatives. The basic idea in the proposed approach relies on substituting the black box modules by metamodels based on a kriging interpolation that assumes that the errors are not independent but a function of the independent variables. A kriging metamodel uses a non Euclidean measure of distance that avoid sensitivity to the units of measure. It includes adjustable parameters that weight the importance of each variable getting a good model representation, and it allows to calculate errors that can be used to establish stopping criteria and provide a solid base to deal with 'possible infeasibility' due to inaccuracies in the metamodel representation of objective function and constraints. Jose has proposed a detailed algorithm that continues with refining stages and successive bound contractions in the domain of independent variables with or without kriging recalibration until an acceptable accuracy in the kriging metamodel is obtained. While in general it is not possible to guarantee convergence to a local optimum of the rigorous nonlinear model, Jose has identified sufficient conditions that rely on a trust region approach, which however is computationally only feasible for low dimensionalities (up to 5 decision variables). Jose has successfully applied his method to a small analytical example, two distillation problems that make use of the simulator HYSYSand optimize the vapor flows, and a flowsheet for producing phthalic anhydride from o-xylene where a plug flow reactor is replaced by a kringing model. In all cases encouraging results were obtained. The paper that was listed in the previous newsletter has been accepted.

Synthesis of Crystallization Processes

New developments: Accepted manuscript

Post-doctoral fellow: Ricardo Lima (started July 2006)

Ricardo has addressed the optimization of the separation of p-xylene from a mixture of mixed xylenes using crystallization. Ricardo proposed a superstructure that is a generalization of the flowsheets studied by Carlos Mendez et al. (2005). Ricardo has embedded all the flowsheets studied by Carlos and considered new connections between stages. The superstructure includes a sub-superstructure for the first crystallization stage and a new sub-superstructure for the set of centrifuges with wash, which allowed establishing new connections between the different process stages so as to consider flowsheets that have been proposed in US patents. In the MINLP model the integer variables are associated with equipment and with disjunctions related with solubility predictions. To solve this problem Ricardo developed a two-level decomposition consisting of the iterative solution of an aggregated and a detailed model. The two key ideas in the aggregated model are: a) merging the units in centrifuge blocks and slurry drums into single input-output blocks so that the aggregated model is defined in the space of interconnection of major blocks; b) elimination of the constraints that set an upper bound on the inlet flowrate of each centrifuge unit. In this way a large number of equations and variables are eliminated because groups of individual units are replaced by a single equivalent unit. However, in order to meet the same production targets, the constraints that impose operating ranges for the centrifuges are relaxed in the aggregated model. For the definition of the detailed model, the number of units in each aggregated block is calculated by the ceiling of the ratio between the calculated capacity of the block and the upper bound of the size for each unit. At each iteration of the two-level decomposition an integer cut is added to the aggregated model to eliminate previous combinations of number of units. This requires the introduction of binary variables in the aggregated model in order to calculate the number of units associated with each aggregated block. The solution of the aggregated model is used to initialize the detailed model as well as to define a reduced superstructure for the detailed model. Since convergence cannot be guaranteed in terms of lower and upper bounds, we simply iterate over a fixed number of major iterations.

The results obtained show that the aggregated MINLP model is easier to initialize and to solve than the MINLP model of the overall superstructure. Furthermore, the solution from the aggregated model provides

a good initial point for the detailed model. The optimum flowsheet that was obtained yields a new design alternative compared to previous flowsheets studied by Carlos Mendez. Comparing the configuration of the optimum flowsheet obtained by these authors with the one obtained in this work, the latter has three fewer slurry drums, one less melting stage, four fewer centrifuges, but one more crystallizer. This led to a reduction of 12% in the total annualized investment cost but at the expense of a small increase in the total annual operating cost, resulting in a modest net improvement in the total annual profit. Ricardo has had this manuscript accepted in AIChE J. A copy can be found in the list below.

Design for Sustainability

New development: **Two manuscripts were completed**

Post-doctoral fellow: **Gonzalo Guillen**

Gonzalo, a postdoc with a Fulbright fellowship, and currently a faculty member at the University Roviri e Virgili in Tarragona, has incorporated sustainability considerations in the synthesis and design of chemical processes. The aim of this work has been to develop tools based on mixed-integer modeling techniques that can facilitate the adoption of more sustainable alternatives for a wide range of problems arising in PSE.

Gonzalo has developed a holistic framework for the design of sustainable chemical supply chains that takes into account the uncertainty associated with the impact assessment model. The environmental impact is measured through the Eco-Indicator 99, which reflects the advances in the damaged oriented method recently developed for Life Cycle Impact Assessment. This strategy covers the entire life cycle of the product, process or activity, including extracting and processing of raw materials; manufacturing, transportation and distribution; reuse and maintenance; recycling and final disposal. The strategy proposed by Gonzalo explicitly considers the uncertainty associated with the emissions used for the damage model for Life Cycle Assessment. Specifically, the variability of the Eco-Indicator 99 under the uncertain environment is controlled by reducing the probability of exceeding a specified target level. Gonzalo formulated this problem as a bi-criterion mixed integer linear program. The objectives are maximizing the net present value (NPV) and minimizing the probability of an Eco-Indicator 99 value below a given target. The inclusion of the latter criteria gives rise to a chance-constraint whose deterministic equivalent is obtained by applying concepts from chance-constrained programming. The resulting multi-objective model is reformulated as a parametric MILP. The probability associated with the Eco-Indicator 99 is treated as the main objective whereas the NPV is constrained to be greater than an epsilon value. By parametrically changing this epsilon value, the entire set of Pareto optimal solutions of the problem can be generated. The parametric MILP is solved by decomposing it into two sub-problems and iterating between them. The first sub-problem is a parametric LP obtained by fixing all the binary variables of the original formulation. This problem is solved by performing a sensitivity analysis with respect to the target imposed to the NPV. This yields a parametric profile that is intersected with the current best one providing an approximation to the Pareto curve of the original problem. The second sub-problem is a MILP where the epsilon parameter is relaxed as a variable. This MILP includes parametric cuts and logic cuts that are derived from previous explored solutions. The parametric cuts force the model to seek solutions improving the best current parametric profile in at least one point. The logic cuts are added to exclude the solutions found in previous iterations. Using the proposed model and solution procedure Gonzalo solved several case studies related to a supply chain in Tarragona, Spain, with possible expansions and distributions in Central Europe. The results show how environmentally friendlier solutions in the face of uncertainty in the damage model can be obtained by systematically trading-off the economic benefit of the process. These robust solutions are achieved by structural modifications in the SC and also by properly adjusting the production rates and transportation flows between the SC nodes. Furthermore, the proposed decomposition strategy is able to provide the whole set of Pareto optimal solutions in a fraction of the CPU time required in the standard epsilon-constraint method. Gonzalo completed a manuscript on this work which has been accepted in *AIChE J*.

Gonzalo has extended this technique to account for uncertainty in the coefficients that are used in the damage model of the Eco-indicator 99. The difficulty here is that the approach of using the chance

constraint for minimizing the probability of an Eco-Indicator 99 value below a given target, gives rise to a nonconvex problem. The resulting bi-criterion non-convex MINLP has been solved by applying the epsilon constraint method. To guarantee the global optimality of the Pareto solutions, Gonzalo developed a novel branch and bound strategy that exploits a number of mathematical properties such as relating the original objective which is non-convex to a simplified objective that has a unique solution. Furthermore, he has also shown how to obtain in a clever way a tight upper bound. He rigorously proved several properties that form the basis of the algorithm. The method was also successfully applied to similar problems as the one in the first paper. The manuscript on this work has been submitted to Computers & Chemical Engineering.

Design and Planning of Deep-Water Oilfield Development under Uncertainty

New Developments: **Preliminary updating scheme for MILPs with changes in the objective**

Students: **Bora Tarhan (Ph.D. started January 2005)**

The project of Bora Tarhan deals with the design and planning of gas and oil fields under uncertainty.

As a first step Bora initially addressed the following stochastic optimization. A network of candidate processes is given over a specified time horizon that is described by multiple time periods in which product demands are specified. It is assumed that major uncertainties are involved in the yields of each process, which are described by discrete probability distribution functions. The uncertainty can be reduced with the potential investment in pilot plants, which delays the introduction of a process but provides more accurate process information on the yields. In addition, once a process is installed, the uncertainties in the yields decrease with time to reflect the experience and improved understanding in the operation of the process. The problem then consists of making planning decisions for process selection, capacity expansions, and possible investment in pilot plants in order to maximize the expected net present value over the specified time horizon. In order to capture all the complex trade-offs, Bora developed a new mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints that are similar in spirit to Vikas Goel's model. One important difference is the time varying uncertainty, which for simplicity Bora considered is revealed over two time periods. Furthermore, he assumed that the time required for a pilot plant study corresponds to one time period. In order to solve this problem Bora developed a dual Lagrangean branch and bound method. Bora successfully applied this method to a 3 process network, with one existing process and two with new technologies and for which investment of pilot plants can be considered over a 10 year horizon. Reformulating this problem as a single MILP involves 7,360 0-1 variables, 8,841 continuous variables and 85,139 constraints. After one week CPLEX obtained a net present value of $61.5 million. With the proposed method a solution of $80.14 was found in 10 hours of CPU time with a gap of 3%. The proposed solution did not select pilot plants to reduce the uncertainty, and proposed expanding Process I up to a capacity of 10 tons/day and making an additional expansion of 4.49 tons/day at time period 1 if the yield turns out to be 69%. If the yield for Process I is found to be 81% then an expansion of 2.98 tons/day is made also at the time period 1.

For the deep-water oilfield development problem, Bora has considered an oil field consisting of a number of reservoirs where each contains several possible well sites. Some of these well sites have to be drilled and exploited for oil over a planning horizon. The oil field infrastructure can be composed of Floating Production Storage and Offloading (FPSO) and/or Tension Leg Platform (TLP) facilities. The FPSO facility can be either a small FPSO, converted from a retiring oil tanker, or a large FPSO, newly constructed grassroots facilities. An FPSO facility can produce, store and offload the produced oil to other tankers. Unlike FPSO, a TLP facility cannot produce oil; it possesses only drilling and oil recovering capability. TLP and FPSO facilities can be connected to each other through pipes. There are two options for drilling wells: sub-sea well or TLP well. Drilling ships are used to drill sub-sea wells, so there is no need to have an FPSO or a TLP facility present to drill a sub-sea well. A sub-sea well has to be connected to an FPSO facility, whereas a TLP well has to be connected to a TLP facility. The problem consists of selecting investment and operation decisions such as selection of the type, location of facilities, time to build them, selection of wells to drill, the time to drill each well, time to connect each well to the facilities and production from the wells. There are uncertainties in the sand quality, size of the reservoir and

breakthrough time. Given the above assumptions, the goal is to maximize the expected net present value of the project. Bora has developed reservoir model where the oil rate decreases linearly or nonlinearly, and the water-to-oil ratio follows a nonlinear function with the cumulative oil production.

Bora developed an MINLP model and solution method that he has largely completed in his second and third internships at ExxonMobil. He developed a model in which facilities and wells of the original problem are aggregated. Instead of deciding which well to drill or which facility to build, the decisions are how many wells or facilities to build. Bora initially modeled the production profile (deliverability vs. cumulative production) as a linear function but in the last few months he has incorporated a more realistic nonlinear model that in principle one might fit with the results of a detailed reservoir simulation model. To account for the fact that uncertainties are not revealed immediately, Bora incorporated a number of rules that specify when the uncertainty is revealed, either in terms of number of items (e.g. number of wells) or in terms of time of production. Because of the aggregation, variables for connection of facilities and wells are disregarded, and lengths to wells are underestimated in order to guarantee that the model predicts an upper bound on the detailed model. This model is similar to the process networks model with the exception that each scenario is a non-convex MINLP. The steps of the algorithm are the same, except that each subproblem is solved using BARON as the global optimization algorithm, although Bora is also testing the use of DICOPT as it is much faster but without guarantee of global optimality. The relaxation yields an upper bound and the lower bound is generated by a simple heuristic. At this point Bora has implemented the method using a special scheme for subgradient optimization to update the Lagrange multipliers. He has recently considered the case of one reservoir with linear production profile over a 10 year period. The best feasible solution is obtained on an example that had an expected NPV of 6.5×10^9. In the optimal solution, the model predicts start building two small FPSO facilities and drill 9 subsea wells. Depending on the future outcomes the investments range from building up to 21 TLPs and 8 additional small FPSOs (best case) to only drilling subsea wells (worst case). This solution was shown to have a significantly higher expected NPV compared to the deterministic solution (NPV=4.4×10^9). Bora is close to completing the manuscript of this work.

In addition to the above work Bora has been investigating the problem of how to most effectively update the successive MILPs that are involved in the solution of the Lagrangean subproblems. An interesting feature is that only the coefficients in the objective function are changed at each iteration. The question is then to see if one can determine a-priori the maximum change in the objective given the updated values of the multipliers. If the change is small, then one can of course omit the solution of the MILP. Bora has developed an initial version of a method that relies on using concepts of sensitivity analysis for MILP and that have been developed by John Hooker. Basic idea is that one can develop a set of inequalities that predict changes in the objective for changes in the coefficients of the objective. These inequalities are applied at terminal nodes of the branch and bound tree to predict the maximum change in the objective. Bora has results for very small problems, but they look encouraging.

Mutisite Planning and Scheduling of Multiproduct Plants

New developments: Spatial and temporal Lagrangean decomposition

New student: Sebastian Terrazas Moreno [Ph.D. started on Jan 2008]

Sebastian is a new Ph.D. student who in general terms is following the line of work by Muge Erdirik and who will collaborate with Dow Chemical. The initial problem that he has addressed for his Ph.D. qualifier deals with the optimal planning of production and distribution activities in a network of continuous multiproduct manufacturing sites that supply a set of common products to a variety of markets. The problem involves deciding which products to manufacture in each site, how much to ship to each market and how much to keep in inventory to satisfy future demand. The objective is to maximize profit. Each site has different production capacities for each product and different operating costs. Product demands are different for each market, and shipping costs between markets and sites can vary significantly. Production and distribution planning is concerned with mid to long-term decisions usually involving several months, adding a temporal dimension to the spatial distribution given by the multi-site network. In addition, there

are significant sequence dependent changeovers every time one switches from the production of one product to another.

Using as a basis the MILP model that Muge developed for her Ph.D. work, Sebastian developed a multiperiod mulitisite MILP model that allows for the possibility of production shut-downs. Since the resulting MILP can quickly become intractable, Sebastian has investigated the use of Lagrangean decomposition, exploring both spatial and temporal decompositions. In order to provide for a framework on deciding between the two, Sebastian formulated a model that introduces new duplicate variables for the coupling constraints (spatial and temporal) in both schemes, with corresponding equalities for the new variables. Using as a basis this model, Sebastian has shown that one can solve the relaxed LP to compute the multipliers for the new equality constraints. These in turn can be used to predict which scheme will yield a smaller increase in the objective when the corresponding coupling equations are relaxed and dualized in the objective function. Reason one would prefer a smaller increase in the objective is to obtain the tightest bound on the profit when applying Lagrangean decomposition. Sebastian also explored the use of subgradient optimization versus the use of cutting planes when solving the dual problem, and developed a hybrid scheme that starts with the former and terminates with the latter. On a problem with 6 sites, 6 market, 6 months, 6 products (252 0-1 vars., 10,621 cont. vars., 9463 constraints) the full space problem could not be solved to optimality after 10,000 secs of CPU time with CPLEX 10.2. The temporal decomposition converged after 800 secs with a 4.2% gap, while the spatial decomposition required 5489 secs with a larger gap of 13.6%. The superiority of the temporal decomposition was confirmed by analyzing the one norm of the corresponding Lagrange multipliers (171 for temporal vs. 1175 spatial). One of the aims of Sebastian has also been to see if one can theoretically prove that temporal decomposition is always superior, which is a conjecture that we believe is true.

Design and Planning of Responsive Supply Chains

New Development: **Completed and submitted paper on probabilistic inventory for safety stocks**

Students: **Fengqi You [Ph.D. started Jan 2006]**

The goal of this project, which is being performed in the context of the Enterprise-wide Optimization initiative, is to develop a comprehensive optimization model that allows the effective integration of long term strategic design decisions for multisite process manufacturing facilities, with short term planning for production and distribution that accounts for the time delays and inventories across the supply chain. The motivation is that most optimization models assume that material can be transferred instantaneously. In that way lead times, or response times once orders are placed, are not taken into account. It is our major goal to establish the trade-offs between economics and deterministic and probabilistic lead times.

As a first step Fengqi addressed the long term design problem of a supply chain, for which he developed a superstructure model that involves both dedicated and multiproduct continuous plants. The time horizons considered are of the order of years, and no inventories are considered, which qualitatively corresponds to the worst case for deterministic lead times. The problem is posed as a bi-criterion optimization problem in which the objectives are to maximize net present value and to minimize lead time. To reflect lead times for different choices of topologies Fengqi considered constraints that measure the duration of the longest time path of chemical flows from a supplier to a customer by way of manufacturing sites. The proposed constraints involve transportation times and residence times in processes. For dedicated plants the times are simply constants, while for multiproduct plants they correspond to cycle time plus residence time minus its processing time. Note that the cycle time results from a scheduling optimization that has to be accounted for. In the case of dedicated plants the problem can be formulated as an MILP, since nonlinear terms defining the lead times can be linearized. For the case of multiproduct plants, the model leads to a nonconvex MINLP problem. Fengqi obtained results on a production network for polystyrene resins that involves a dedicated process (styrene), and two multiproduct plants (solid polystyrene and expandable polystyrene). Three potential plant sites are considered, with two suppliers, and up to 5 customers For 3 time periods (2, 3 and 5 years) the model involved 133 0-1 variables, 2249 continuous variables and 3041 constraints. To develop the trade-off curve the ε-constraint method was used. DICOPT required 3.5

minutes while BARON required about 100 hours. The solution involving shortest lead time of 8.85 days had an NPV of $158 million, while the longest lead time was 14.42 days at a much higher NPV of $1,261 million.

Fengqi extended the above problem to a probabilistic model for stockout. In this way instead of using a deterministic lead time that only relies on transportation and production times with zero-inventory, Fengqi proposed an expected lead time that represents the expected value of time delays incurred by transportation and production across the supply chains, and accounting for inventories in the distribution centers. This expected lead time is then used as a quantitative measure of supply chain responsiveness. This probabilistic model for the safety stock levels accounts for demand uncertainty. This probabilistic constraint is reformulated as deterministic constraints for which Fengqi obtained analytical expressions for the triangular and the normal distributions of the demands. The bi-criterion optimization model was also solved with the ε-constraint method, but Fengqi has also developed a hierarchical algorithm for the solution of the resulting large-scale MINLP problem that is based on decoupling of the decision-making levels (strategic and operational). Fengqi solved two examples related to the styrene problem described above. The results show that small changes in expected lead time can lead to significant changes in the net present value and the network structure, which in turn suggests the importance of integrating responsiveness into the design and operations of process supply chain network. An interesting by-product of the model is a trade-off curve of safety stock versus expected lead time, which provides very useful information. Fengqi has completed a manuscript on this work which has been accepted by Computers & Chemical Engineering.

Supply Chain Optimization under Uncertainty

New Development: Risk management for global chemical supply chain operations
**   Capacity planning with reactor transformation and construction lead time**

Students: Fengqi You [Ph.D. started Jan 2006]

This is a new project collaborated with Dow Chemical in the context of the Enterprise-wide Optimization. The major goal is to develop optimization models and algorithm for chemical supply chain optimization under various types of uncertainties and risks. Based on an internship at Dow Chemical in Midland, Fengqi addressed the risk management for supply chain operations under uncertainty, a case study that was selected by Dow for the EWO project. In this work, Fengqi worked with John Wassick to develop a two-stage stochastic linear programming approach for the tactical planning of a global multi-product chemical supply chain that is subjected to uncertainties in production reliability and customer demands. Monte Carlo sampling and the associated statistical methods are applied and incorporated into the stochastic programming model to avoid the large number of scenarios required. A simulation framework was also developed to assess the potential improvement of using stochastic programming in the supply chain planning process compared with traditional deterministic approaches. The results of the case study show that on average cost savings of 5.70% could be achieved by using the stochastic programming model on a monthly basis. To solve the large scale case study effectively, a multi-cut L-shaped solution method is developed that can achieve significant savings in CPU times. To explicitly consider the risks included in the global supply chain planning process, Fengqi studied four risk management models by using different risk measures. A real world case study was presented to demonstrate the effectiveness of the proposed models and algorithms. Computational studies suggest that probabilistic financial risk management model and downside risk management model are more effective in reducing high cost risk compared with the popular variance management and variability index management models. Fengqi has completed a manuscript on this work which has been submitted for publication and is available to CAPD members.

As a second step, Fengqi considered a project on capacity planning with reactor transformation, which is also provided by Dow Chemical in the context of the Enterprise-wide Optimization. In this problem, we are given a production-distribution system with a number of production sites and customers. Each production site has some production trains. We are also given a number of products that can be categorized into a few product families. There are some types of production trains available, and each type of production train can produce a certain given product family. The actions of capacity modification includes adding a new

production train in a new or existing production site, removing an existing production train, and convert an existing production train from producing one product family to producing another product family. Construction lead times for each capacity modification actions are given and should be taken into account. As a first step, Fengqi developed an MILP model for the deterministic case. A resulting challenge is that the MILP model has a large number binary variables and logic constraints due to the "reactor transformation" constraint. Fengqi is now working on developing an efficient algorithm to solve the large scale MILP problem. Fengqi is also working on is to address demand uncertainty for this problem.

Integrated Supply Chain Design and Stochastic Inventory Management

New Development: **Lagrangean decomposition for joint location-inventory model**
                        Large-scale supply chain design with multi-echelon stochastic inventory

Students: **Fengqi You [Ph.D. started Jan 2006]**

Optimizing inventories across the supply chain has become an emerging challenge for the process industries to reduce costs and improve the customer service. This challenge requires integrating inventory management with supply chain network design, so that decisions on the locations to stock the inventory and the associated amount of inventory in each stocking location can be determined simultaneously. Fengqi has been working on a classical operations management problem for joint location-inventory problem inspired by the work of Shen, Coullard, and Daskin (2003). The problem is as follows. The locations of the supplier and the customers are known and the distances between them are given. The supplier to customers lead time is assumed to be the same for all the customers. A number of candidate sites are given to locate the distribution centers (DC), and there are fixed setup costs when distribution centers are established. Each customer has a normally distributed demand which is independent of other customers' demands. Each DC can connect to more than one customer, but each customer should be only assigned to exactly one distribution center to satisfy the demand. Linear transportation costs are incurred for shipments from supplier to DC and from DC to customer. Most of the inventory in the network is held in the DCs, where the inventory is managed with a (Q, r) policy with type I service. Inventory costs are incurred at each DC and consist of working inventory and safety stock. The customers only maintain a small amount of inventory whose costs are ignored. The objective is to determine how many DCs to locate, where to locate them, which customers to assign to each DC, how often to reorder at the DC, and what level of safety stock to maintain to minimize the total location, transportation, and inventory costs, while ensuring a specified level of service. Fengqi first reformulated the model as an MINLP problem. Using its convex relaxation model for preprocessing, he developed a local optimization heuristic method to obtain near-global optimal solutions very quickly. Based on this model, Fengqi also proposed a Lagrangean relaxation and decomposition algorithm for the global optimization of the model. He obtained numerical results for examples ranging from 33 to 150 customers. Fengqi has completed a manuscript on this work which has been accepted by "Industrial & Engineering Chemistry Research" and is available to CAPD members.

As a second step, Fengqi has extended the above problem for supply chains with multi-echelon inventory systems in the presences of uncertain customer demands. By using the guaranteed service approach (Graves and Willems, 2000) to model the multi-echelon stochastic inventory system, the stochastic nature of the problem is captured and imbedded into an equivalent optimization model for simultaneously optimizing the transportation, inventory and network structure of a multi-echelon supply chain under demand uncertainty. The model determines the supply chain design decisions such as the locations of distribution centers (DCs), assignments of each downstream node to its upstream node, shipment levels in each arc of the supply chain network, and inventory decisions including the pipeline inventory and safety stock in each node of the supply chain network. The model also captures risk-pooling effects by consolidating the safety stock inventory of downstream nodes to the upstream nodes in the multi-echelon supply chain. Fengqi first formulated this problem as an MINLP with a nonconvex objective function including bilinear, trilinear and square root terms. By exploiting the properties of the basic model, Fengqi reformulated the problem as a separable concave minimization program. A tailored spatial decomposition algorithm based on Lagrangean relaxation, piecewise linear approximation and the model property is developed to obtain near global optimal solutions (below 1% gap) with reasonable computational expense. Two examples on industrial gases supply chain and performance chemical supply chain are presented to illustrate the applicability of

the proposed model. Computational examples for industrial gas supply chains with up to 5 plants, 100 potential distribution centers and 200 customers are presented to illustrate the performance of the algorithm. Fengqi is completing a manuscript on this work.

Stochastic Vehicle Routing and Tank-sizing

New Development: Continuous approximation model for capacitated inventory-routing problem

Students: Fengqi You [Ph.D. started Jan 2006]

This is a new project in collaboration with Praxair in the context of the Enterprise-wide Optimization. The objective is to optimize asset allocation in the merchant liquid supply chain by incorporating operating decisions. Specifically, given is a set of customers over a long time horizon (typically 5 years). The problem is to determine the optimal fleet and storage capacity allocation over time with the objective of minimizing capital and operating costs. Fleet capacity can be reallocated and increased in the short term by converting trailers from one product to another and/or by hiring third party carriers and in the long term by acquiring new fleet. Storage capacity can be modified by relocating and installing new tanks at storage facilities and at customers. An inventory of discrete size tanks may be available. A major feature of this problem is that Praxair manages inventory for the customers, i.e. it determines who receives a delivery each day, by which route and what the size of that delivery is. Thus, the distribution planning problems associated with such vendor managed re-supply policies are known as inventory routing problems (IRP). The typical objective of an IRP is to minimize operating (distribution and inventory) costs. Even though the IRP is a long-term problem, almost all proposed solution approaches solve only a short-term version of the problem to make it easier.

To integrate the long term strategic tank sizing decision with the short term routing decisions, Fengqi has developed a continuous approximation model for this problem. The basic idea to approximate the capacitated vehicle routing or delivery cost in the strategic level, so as to tradeoff the inventory capital cost (tank sizing). Computational results on a toy problem have shown that the CPU time can be reduced from around 20 minutes by using the detailed integrated model to 20 seconds by using the continuous approximation model with the same optimal solution on tank sizing. Fengqi is now working on the stochastic version of this problem. Uncertainties from demand fluctuations and the loss or addition of customers over time are also being investigated.

Optimal Scheduling of Crude Oil Operations

**New development: Symmetry breaking constraints for new continuous time MILP model
                           and their integration through CP**

Student: Sylvain Mouret [Ph.D. started Jan 2007]

Sylvain, who joined the department in January 2007 from Ecole Polytechnique in Paris, is working on a project funded by Total through the collaboration with Pierre Pestiaux. The specific problem that Sylvain is addressing is the scheduling of crude oil operations in the front-end of a refinery that is composed of crude marine vessels, storage tanks, charging tanks and CDUs. Crude vessels unload crude oil into storage tanks during a time window depending on the arrival time to the refinery. These crude-oils are then mixed into charging tanks before being distilled by CDUs which separate the charged oil into fractions such as gas oil, gasoline, kerosene, heating oil and residues. Given arrival times of marine vessels, capacity limits of tanks, flow rate limitations, initial key components concentrations in vessels and tanks, components concentration ranges as part of distillation specifications, demands for each mixed oil, and a time horizon, the objective is to determine time and volume variables of all crude-oil transfer operations in order to maximize the gross margins of distilled mixed oil.

Sylvain has developed a novel continuous time model for this scheduling problem that relies on the idea of postulating a potential number of tasks (slots) to be executed. The proposed approach consists then of assigning specific transfer operations to the ordered set of slots whose cardinality has to be postulated. The objective used is to maximize the gross margins of crudes that need to be processed to satisfy given demands. By introducing the appropriate 0-1 variables for assignments, as well as precedence constraints that enforce non-overlapping operations (e.g. inlet and outlet of a given tank), the problem can be formulated as an MILP provided the constraints on compositions for blending are relaxed. Once the solution is obtained for this problem, an NLP subproblem is solved with fixed 0-1 variables to enforce the composition constraints. This yields an upper bound, which surprisingly Sylvain has found to be very tight, and in many instances with zero-gap. Sylvain has applied this solution approach to several problems from the Lee et al. (1996) paper obtaining very encouraging results.

One feature in the proposed MILP model, however, is that it has many degenerate or "symmetric" solutions which leads to the enumeration of a larger number of nodes. Sylvain has addressed the symmetry challenge by using a regular language, and its corresponding Deterministic Finite Automaton (DFA), in order to restrict the possible sequences of operations assigned to the set of time-slots. This restriction is can then be added to the model under the form of linear network flow constraints as explained in Côté et al. (2007). Sylvain has also developed an integrated hybrid approach using CP to handle the logic constraints including the symmetry-breaking constraints. This approach consists in use using inference techniques at each node in order to extend the branching decisions to more than one variable whenever it is possible. The hybrid approach has been tested on the 4 instances of a crude-oil operations scheduling problem from Lee et al. (1996.) The results show that, even though the hybrid approach is slightly less performant in terms of reducing the search space, it leads to 60% average improvement in CPU time. This is due to the fact that constraint propagation of logic constraints is much cheaper than solving the node relaxation of a LP containing complex logic constraints. The largest problem had 3 vessels, 6 storage tanks, 4 charging tanks and 3 CDUs. Postulating 30 slots the problem was solved in 560 sec (21 nodes) using the pure MILP approach while it was solved in 146 sec (91 nodes) using the hybrid MILP-CP approach.

The integration of CP has been taken one step further by using it in order to strengthen the linear relaxation of the MILP. CP inference techniques have been used to get tight bounds of continuous variables involved in bilinear constraints at each node. These tight bounds can then be used to generate McCormick cuts (based on McCormick under and over estimators of bilinear terms). This approach has been used on the Lee et al. (1996) problems where the objective is to minimize logistics costs which include storage costs. In continuous-time formulations, storage costs appear in the objective function as bilinear terms (volume * storage duration), thus resulting in poor linear relaxations (relaxation gap over 100%). The use of CP has allowed reducing the optimality gap in this case to less than 15% while keeping the computational expense small.

Planning of Refinery Operations

New development: **Modeling steam stripping column**

Student: **Abdulahraman Alattas [Ph.D., started Jan 2007]**

Abdul's project is a joint collaboration with BP through Ignasi Palou-Rivera in the Enterprise-wide Optimization project. The major objective is to develop refinery planning models that incorporate nonlinear process models, in contrast to the common fixed yield models that lead to robust LP models that are prevalent in industrial practice (e.g. PIMS).

The specific problem that Abdul is addressing is for complex refinery configurations for processing heavy crudes. The crude is introduced into the crude distillation unit (CDU) that combines the atmospheric distillation column and the vacuum distillation column and produces the first cuts of the crude. These include the overhead fuel gas, straight-run naphtha, straight-run gasoline, straight-run light distillate, straight-run gas oil and the bottom residue. Along with the CDU, the configuration of interest includes the following process units: naphtha reforming unit that produces reformed gasoline and fuel gas from straight-

run naphtha, catalytic cracking unit that produces fuel gas, gasoline and fuel oil from straight-run light distillate and straight-run gas oil, residue hydrotreating unit that treats the bottom residue to blending quality, and product blending units that combine different intermediate product streams to produce the desired final products: premium gasoline, regular gasoline, diesel, fuel oil and residue. The objective of the planning model is to determine the types, quantities and mixing strategies for the different crude oils available for purchase, so that the refinery will meet the objectives of maximizing profits while meeting specific demands over a specified time period. Abdul implemented both fixed-yield models and swing-cuts models in order to assess their relative benefits. The swing cuts model, which can also be formulated as an LP, can be thought of a model that has the flexibility of transgressing the fixed boundaries of the fixed yields models within certain limits. In a specific instance Abdul found that thee swing cuts model can predict a solution with 10% improvement in the profit, largely due to different decisions in the purchase of crudes.

In the last few months Abdul has implemented an extension of the aggregate distillation models proposed by Jose Caballero. This requires that the CDU be represented through cascaded columns, including columns with steam stripping. A direct implementation of the aggregate model on a mixture between 10 and 20 hydrocarbons and with conventional distillation columns led to significant convergence problems, often yielding infeasible NLP solutions. In order to improve the convergence, Abdul derived valid linear inequalities for the flows of vapor and liquid, since these obey complex relations given the thermal integration of streams in the cascaded columns. These inequalities significantly improve the robustness of the solution of the NLPs. Abdul has been able to solve up to 4 cascaded columns with up to 20 components. The next major step has been to replace on the cascaded columns by one with steam stripping. Initial attempts to use several common models were not successful in overcoming convergence problems. Therefore, Abdul has been developing a simplified aggregate model that treats the steam as an inert component and that can reproduce the effect of having an inversion of temperature (i.e. bottoms lower temperature than feed temperature). The main idea is to account for the changes in the vapor pressure at the bottom and feed. Calculations on the individual steam stripper have proved to be fairly accurate. We expect that this model will be successfully implemented as part of the cascaded columns. Another future direction will be to make use of pseudo-properties for handling real crudes.

Planning for Petroleum Allocation

New development: **Disjunctive decomposition**

Post-doctoral fellow: **Roger Rocha [started September 2007]**

This project involves Roger Rocha from Petrobras who is visiting for two years. The main objective of this work is to investigate a mathematical programming approach to solve the Petroleum Allocation Problem at Petrobras. Petroleum allocation must be programmed so that sufficient supplies of required crude oil reach refineries along the planning horizon. This must be done by taking into account strategic planning and operational constraints along the petroleum supply chain as follows. Crude oil can either be locally produced or imported from abroad. Local crude oil comes from production sites, mostly offshore, and is transported either by tankers or pipelines. Imported oil is only transported by tankers. After reaching maritime terminals, crude oils are either exported or shipped to Petrobras refineries. At the refineries, petroleum is processed in crude distillation units (CDUs) on daily scheduled production campaigns. These campaigns are defined by consumption rates of different petroleum categories, duration, release date, and deadlines to completing them. Roger proposed an MILP formulation of the problem which relies on a time/space discretization network. The formulation involves some inequalities which are redundant to the mixed integer model but not necessarily to LP relaxation. As the model itself was not able to solve industrial size instance of the problem, not even to find a feasible after 15 days of computation, he implemented a heuristic to find an initial feasible solution by fixing some variables associated with the hardest part of this model and solving the remaining part. In order to improve the solution quality we use a local search method by optimization called local branching, that in most of the case studies could find a solution guaranteed to be no more than 10% of optimality in less than 5 hours.

Roger developed some valid inequalities which are associated with polytopes that have been extensively studied in the literature. Furthermore, separation routines for strong valid inequalities associated with these polytope are readily available in some commercial solvers. Use of this feature allows a substantial reinforcement of the underlying LP relaxation to be attained. He has tested on some industrial-size instances of the problem involving approximately 40 crude oils, 6 tanker types, 8 maritime terminals involving 12 docks, 11 refineries, and 21 crude distillation units over a time horizon of 72 discretized intervals. Typical instances have 40,000 binary variables, 160,000 continuous variables, and 40,000 constraints. He presented this work at the FOCAPO meeting.

In a new exciting development Roger has developed a decomposition scheme for problems that can be decomposed into subproblems. The idea is to duplicate variables as one would do in Lagrangean decomposition, but the entire objective is transferred only to the first subproblem while the remaining ones are defined as feasibility subproblems. In the next step disjunctive cuts are generated for the subproblems. Instead of simply using these constraints as cuts, the idea is to use valid inequalities for disjunctions and generate cuts through the reverse polar as per the work by Egon Balas. Roger has tested this idea in the now classic batch scheduling problem of parallel lines by Vipul Jain. Roger has applied his method to this problem and obtained very good results showing that his cuts are stronger than the combinatorial cuts that had been developed by Vipul. Roger is currently implementing his ideas to solve the large Petroleum Allocation Problem.

Cost model for a multiproduct process with multiple stages

Post-doctoral fellow: Ricardo Lima [started July 2006]

Ricardo started a new project with the Glass Technology Center (GTC) from PPG Industries with the aim of developing a mathematical model for the cost estimation of the value added magnetic sputtering vapor deposition (MSVD) coated and tempering glass products. These products are manufactured in a multiproduct plant with multiple stages. The products are defined by different substrates and dimensions. The work involved in a first stage the identification of the operating costs associated with all the stages, raw material and transportation costs, and in a second stage the mathematical formulation and implementation of cost functions. Different scenarios were considered and optimum policies suggested, accounting for different cutting strategies and number of pieces per batch. The cost model allowed the estimation of the partial and final costs of more than 600 products. In addition, the profit of each product was also estimated and both were compared with standard variable costs and profits used by PPG Industries. This comparison provided valuable information about the accuracy of the cost estimation software. The systematic calculation of such a large number of products allowed conducting studies related with the production flow, namely identification of production losses, inefficiencies, and weight of each operation in the final cost. The final model implementation revealed to be a useful tool for the definition of future market prices.

Ricardo is just beginning a new project with the GTC, PPG Industries related with the planning and scheduling of a multiproduct continuous plant.

Scheduling of Batch Multiproduct Plants

New Development: **Publication of paper for simultaneous batching and scheduling**

Collaboartors: **Pedro Castro (INETI, Portugal)**

Pedro Castro has been collaborating with us for a number of years, especially in light of his postdoctoral stay in 2004-2005. He has mostly devoted his efforts to continuous time RTN models, and to developing effective computational strategies for effectively solving MILP models for large scale scheduling problems.

More recently Pedro, with input from Muge, has a new mixed integer linear program (MILP) for the optimal short-term scheduling of single stage batch plants with sequence dependent changeovers and

optimal selection of the number of batches to produce. It is a continuous-time formulation employing multiple time grids that is based on the resource-task network (RTN) process representation. The main novelty is that aggregated processing and changeover tasks are considered that account for the time required to produce all batches of the product, plus the changeover time to the next product in the sequence. The performance of the new formulation was studied by Pedro through the solution of 12 example problems for the objective of revenue maximization and 4 for the objective of makespan minimization. The same problems were solved by a multiple time grid implicit batching approach, by a continuous-time model with global precedence sequencing variables, by a model with immediate precedence sequencing variables that does not determine the timing of events, and by a constraint programming model. The new formulation emerged overall as the best performer for the scenario of maximum plant flexibility, where different batches of the same product can be produced in different units. The model developed by Muge with immediate precedence sequencing variables was the fastest but it is not a general scheduling model in the sense that it assumes a single cyclic schedule in each unit, which can be broken, but two or more cyclic schedules per unit may result. In such cases, subtour elimination constraints can be added and the problem solved iteratively to find a feasible schedule at the likely expense of removing the global optimal solution from the feasible space. When compared to the implicit batching approach, the computational effort of the new formulation was typically one order of magnitude lower, which in practice indicates that the new formulation can tackle larger problems. When compared to the traditional approach of considering a single processing task per batch, fewer event points are needed, which results in significantly lower computational effort as illustrated through the solution of several example problems. A manuscript describing this work has been published and is provided as a reprint.

Simultaneous Scheduling and Control

New development: **Simultaneous design, scheduling and control of a Methyl-Methacrylate Continuous Polymerization Reactor**

Collaborator: **Antonio Flores-Tlahuacac (Professor U. Iberoamericana)**

This is a collaboration with Antonio Flores from the Universidad Iberoamericana (Ignacio's alma mater). Antonio, being a control person, has been motivated by the idea of using dynamic models for control in scheduling problems. Given our interest in the area of scheduling, we decided to join forces in a work in which the basic idea is to combine a scheduling optimization model, with a dynamic model for the optimization and control of the transitions. In this work we addressed the simultaneous scheduling and control problems for a continuous stirred tank reactor (CSTR) that produces multiple products within a cyclic schedule that involves sequence dependent transitions. The scheduling part of the model is similar to our previous work with Jose Pinto. Because, dynamic profiles of both manipulated and controlled variables are also decision variables, the dynamic part of the model is formulated with DAEs. The resulting problem can then be cast as a Mixed-Integer Dynamic Optimization (MIDO) problem in which the objective function includes income from sales of products, inventory costs and transition costs that takes into account through quadratic deviation terms, the amount of off-specification material produced during product transition. To solve the MIDO problem it is transformed into an MINLP using orthogonal collocation, where initial guesses on the duration of the transitions must be provided. These are then revised in a subsequent optimization. Antonio and Sebastian Terrazas-Moreno subsequently developed a new MINLP formulation to simultaneously solve the scheduling and control problems in polymerization reactors during a cyclic manufacturing operation. In contrast to the previous model, the problem need not be solved sequentially by iteratively assuming fixed lengths for the duration of the transitions. Another interesting feature of the model is that by assuming that the performance of each polymer is only dependent of the initial conditions, the problem can be formulated in terms of 0-1 variables for assigning products to slots. The transitions are then simply computed from the difference in the initial conditions. This leads to a much smaller number of 0-1 variables compared to the case when sequence dependent transitions are explicitly modeled.

In another work, Antonio in collaboration with Sebastian Terrazas addressed the simultaneous scheduling and control (SSC) problem using Lagrangean Decomposition as presented by Guignard and Kim. The

model was decomposed into scheduling and control subproblems, and solved using a heuristic approach used before by Sarette Van den Heever in oilfield problems. The method was tested using a Methyl Methacrylate (MMA) polymerization system, and the High Impact Polystyrene (HIPS) polymerization system, with one continuous stirred-tank reactor (CSTR), and with complete HIPS polymerization plant composed of a train of seven CSTRs. In these case studies, different polymer grades are produced using the same equipment in a cyclic schedule. The computational times in the first two examples were lower for the decomposition heuristic than for the direct solution in full space, and the optimal solutions found were slightly better. The example related to the full scale HIPS plant, which involved 16 0-1 variables and 22,700 variables, was only solvable using the decomposition heuristic. The manuscript describing this work has been published and is available in the next newsletter.

Finally, in recent work Antonio and Sebastian developed a Mixed-Integer Dynamic Optimization (MIDO) formulation for the simultaneous process design, cyclic scheduling, and optimal control of a Methyl Methacrylate (MMA) continuous stirred-tank reactor (CSTR). Different polymer grades are produced in terms of their molecular weight distributions, so that state variables values during steady states are kept as degrees of freedom. The corresponding mathematical formulation includes the differential equations that describe the dynamic behavior of the system, resulting in a MIDO problem. The differential equations were discretized using the simultaneous approach based on orthogonal collocation on finite elements, rendering a Mixed Integer Non-Linear programming (MINLP) problem where a profit function is to be maximized. The objective function includes product sales, some capital and operational costs, inventory costs, and transition costs. The optimal solution to this problem involves design decisions: flowrates, feeding temperatures and concentrations, equipment sizing, variables values at steady state; scheduling decisions: grade productions sequence, cycle duration, production quantities, inventory levels; and optimal control results: transition profiles, durations, and transition costs. Antonio and Sebastian formulated and solved the problem in two ways: as a deterministic model and as a two-stage programming problem with hourly product demands as uncertain parameter described by discrete distributions. The paper describing this work has been completed and is available to the CAPD members.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: Rosanna Franco (started July 2006)

Rosanna Franco has been working on the web-interfaces that are available in:
http://newton.cheme.cmu.edu/interfaces

Rosanna has completed the new interface WATERNET that implements the model by Ram Karuppiah for optimizing the integrated network for water reuse and distributed treatment.

The current list of programs that we have available, most of them in our website, are the following: (description in http://egon.cheme.cmu.edu)

Synthesis:
SYNHEAT   MINLP synthesis heat exchanger networks (Yee)
                      Also includes transshipment model for targeting (Papoulias)
STEAM   MINLP Model for the synthesis of combined cycles for utility plants (Bruno)
                      Model includes correlations for steam, efficiencies and cost data
GLOBESEP   Global NLP optimization for synthesis of separation networks and
                      single feed/mixed products (Quesada)
WATER   Global NLP Model for synthesis of wastewater treatment configuration (Galan)
EXTRACTOR Disjunctive MINLP for synthesis of liquid-liquid extraction systems (Reyes)
GDP-DISTILL GDP Model for the optimal selection of number of trays and feed tray location in
                      distillation columns using tray-by-tray model (Barttfeld)

Batch design:
BATCHSPC   MINLP and MILP models for multiproduct batch plants
                      single product campaigns (Kocis, Voudouris)

BATCHMPC   MILP model for multiproduct batch plants
                              mixed-product campaigns (Birewar, Voudouris)
Scheduling:
STN   State-Task-Network MILP formulation for scheduling multipurpose batch plants. Both the
             Kondili, Pantelides and Sargent (1993) model and the Maravelias and Grossmann (2003) are
             implemented.
PARALLEL   MINLP continuous multiproduct scheduling on parallel lines
                              Features feasibility preanalysis (Sahinidis)
MULTISTAGE MINLP continuous multiproduct in multistage plants (Pinto)
CYCLE   LP/MILP aggregate flowshop scheduling (cycle time/makespan)
                              Includes loop tracing algorithm (Birewar)
STBS   MILP short term multistage scheduling (Pinto, Bolio)
CRUDEOIL   MILP model for refinery scheduling (Lee, Pinto)
DECAY   MINLP model for scheduling of clean-up of parallel furnaces (Jain)
UTILPLAN   MILPmultiperiod model for utility plants (Iyer)
PRODEV   MILP model for scheduling of tests in new product development (Schmidt, Najimas)
                  MILP for resource scheduling in new product development (Jain, Maravelias)
Planning:
PLANNER   MILP multiperiod model for capacity expansion in process networks
                              (conventional and lot sizing model) (Sahinidis, Norton)
MULTISITE   MILP model for planning the selection of processes and capacity expansion in
                  different geographical location and accounting for transportation costs (Turkay)
GREENPLAN   Bi-criterion MILP model for selection of processes that maximize the net present value
                  and minimize toxicity (Drabbant)
NETCHAIN   Multiperiod MILP for supply chain optimization of multisite facilities with flexible
                  processes, intermittent deliveries, changeovers and inventories (Bok/Iyer)

Nick Sahinidis' Group

THRUST 1—OPTIMIZATION ALGORITHMS, THEORY, AND SOFTWARE

Algorithms and Software for Global Optimization of NLPs and MINLPs

Student: **Ms. Xiaowei Bao (Ph.D. student in Chemical and Biomolecular Engineering at the
                          University of Illinois)**

Collaborator: Mohit Tawarmalani (Associate Professor, Purdue University)

As a result of research that was initiated in 1991, we have developed algorithms and software for global
optimization of NLPs and MINLPs. The main results of this work have been:
- A theory of convex extensions that provides a systematic means for developing the functional
  expression of convex/concave envelopes of nonlinear functions of continuous and integer variables.
- An entirely linear outer-approximation of factorable nonlinear programs. Relying on LP relaxations
  results in a robust solution approach to global optimization.
- A variety of range-reduction schemes for reducing the search space of integer and nonlinear programs.
- Finite branching schemes for concave minimization and two-stage stochastic integer programs.
- The BARON software for the global optimization of NLPs and MINLPs.

Xiaowei Bao last year initiated work on the global optimization of quadratically-constrained nonconvex
quadratic programs. This is a class of optimization problems with applications in various settings,
including facility location, multiperiod refinery scheduling and planning, and circle packing problems. The
approach that Xiaowei is currently investigating relies on branch-and-bound. While standard approaches
relax each nonconvex term separately, Xiaowei is exploring relaxations of entire quadratic constraints.
This past semester, we develop new semidefinite programming relaxations for these quadratic constraints.
Contrary to earlier work, our SDP relaxation is in the space of the original variables and does not increase

the dimension of the problem. As a result, a small number of supporting hyperplanes from this SDP relaxation is sufficient to considerably strengthen the quality of the standard relaxation. We have found that this approach improves BARON's performance on this class of problems by several orders of magnitude.

Nick Sahinidis and **Mohit Tawarmalani** are currently maintaining the BARON software. Ongoing work on BARON involves the development of tighter relaxations for MINLPs, work that is expected to be implemented and made available by the end of this coming semester.

Global Optimization for Problems in Quantum Chemistry

Student: **Mr. Keith Zorn (Ph.D. student at CMU)**

Keith Zorn who joined the group in November 2007 has begun the study of optimization problems in quantum chemistry, in particular Hartree-Fock theory. Quantum mechanics utilizes an explicit description of electron distribution to describe atoms and molecules. Hartree-Fock theory is a branch of quantum chemistry consisting of a series of approximations to the time-independent Schrodinger equation. Typically, Hartree-Fock systems are solved through an iterative Self Consistent Field (SCF) process. SCF, however, is a local solution algorithm that depends upon an initial guess and offers no guarantee of a globally optimal solution. Because of the nonlinear and nonconvex nature of the equations, global optimization is necessary to ensure that the true minimum ground-state energy is discovered. Keith worked on an existing multi-extremal, nonconvex, polynomial programming problem for the calculation of ground-state electronic energy for small, closed-shell, Hartree-Fock systems. The literature has suggested a standard linearization technique based on factorable programming ideas to obtain a lower bound for this problem. Keith has applied the Relaxation Linearization Technique to strengthen the relaxation and expedite solution of the optimization model. Through the introduction of relaxed, redundant constraints before linearization, the root node gap, computational time, and number of required optimization iterations are shown to be significantly reduced.

Global Optimization for Machine Learning Problems

Student: **Mr. Xuan Shi (M.S. student at CMU)**

Xuan Shi, who joined the group in November 2007, is working on applications of global optimization in the area of Machine Learning. One of the central questions in neural computing is how to select the neural network parameters (architecture, activation functions, and weights) so as to obtain the best possible neural network model for a given natural or artificial system. This project considers the problem of determining the global minimum of an error function commonly used for training of neural-networks. This is a highly non-linear problem plagued with multiple local optima. Local search algorithms, such as backpropagation, often result in neural networks that are unnecessarily complex and may overfit the data. The project will involve the computational implementation and testing of an algorithm developed earlier by Voudouris and Sahinidis (unpublished), while, in addition, enforcing the first-order optimality conditions. A general-purpose code will be written in GAMS and a generic interface will be developed in order to facilitate testing of the new training algorithm on a variety of test problems from the Machine Learning Repository at http://mlearn.ics.uci.edu/MLRepository.html. This new training algorithm will be evaluated by comparing it against backpropagation, support vector machines, and other popular learning algorithms.

Algorithms and Software for Black-box Optimization

Student: **Mr. Luis Miguel Rios (Ph.D. student in Industrial Engineering at the University of Illinois)**

This project is currently aiming at a systematic testing of existing derivative-free algorithms that are capable of optimizing black-box problems. Derivative-free optimization is an area of recent interest and rapid growth, fueled by a growing number of applications, especially in the oil and gas, and chemical process industries. The major challenge is that the objective function in many problems is expensive to evaluate, while no bounds or Lipchitz constants are available, and strategies to directly estimate derivative information are impractical or expensive. The most recent systematic testing of derivative-free algorithms for solving problems of this nature was done 10 years ago. **Luis Miguel Rios** has collected 225 test problems from the globallib and princetonlib collections and solved them under different conditions using 18 different black-box solvers. These codes were: Adaptive Simulated Annealing, ASA version 26.23 by Ingber; Solvers APPS, DIRECT, EA, PATTERN, and SOLIS-WETS under Design Analysis Kit for Optimization and Terascale Applications (DAKOTA), Version 4.0, from Sandia National Laboratories; Derivative Free Optimization (DFO), Version 2.0, by Conn, Gould, Toint, and Scheinberg; Multilevel Coordinated Search (MCS), by Huyer and Neumaier; the Nelder-Mead algorithm implemented in MATLAB; Nonlinear Optimization for Mixed vAriables and Derivatives (NOMAD), Cycle 6, by Couture, Audet, Dennis, and Abramson; SID-PSM, Version 0.3, by Custódio and Vicente; and solvers EGO, GLB, GLC, LGO, and RBF under TOMLAB.

The main conclusions from this computational study were that: (a) even obtaining a feasible solution cannot be taken for granted for these problems/solvers, (b) larger problems diminish the chances for obtaining good solutions, (c) LGO and MCS are better, on average, than other solvers, (d) all solvers are 'useful' in the sense that there are at least a few problems for which each solver is best in terms of solution quality.

Current plans in this line of research include the addition of non-smooth problems in the test set collection and the inclusion of additional solvers. Test problems of black-box models from industry are currently sought.

New development: the solvers tested by Luis Miguel have been brought under a unified software interface that allows the user to call any of these solvers through a simple interface. This software platform is currently being tested and will be soon made available.

Algorithms and Software for Linear Optimization Problems (LP) and Extensions

Students:
>   **Mr. Deepak Channamariyappa (M.S. student at CMU)**
>   **Mr. Joseph Elble (Ph.D. student in Industrial Engineering at the University of Illinois)**
>   **Mr. Yiqi Zhu (M.S. student at CMU)**
>   **Dr. Panagiotis Vouzis (postdoctoral researcher at CMU)**

Algorithms for solving LPs represent the workhorse of optimization systems for solving large-scale MILPs, NLPs, and MINLPs. While highly successfully commercial software exist for solving LPs, none is guaranteed to provide reliable results in the sense that they are all subject to the effects of floating point arithmetic and round-off errors. The goal of this project is to develop new simplex algorithms and software in order to provide tools that can reliably solve large-scale linear optimization problems even in the presence of round-off errors. Towards this goal, we plan to develop symbolic algorithms for linear programming preprocessing, matrix scaling, and matrix factorization.

The long-term goal of this project is to develop novel algorithms for LPs and make them available via distributed implementations on modern GPUs and FPGAs.

Deepak Channamariyappa has begun the study of preprocessing techniques for Linear Programming. These techniques currently represent more of an art rather than science in the field of Linear Programming. The main goal of Deepak's project is to implement and compare the computational performance of different preprocessing techniques. It is expected that this study will be beneficial for the development of

useful tools for nonlinear optimization problems as well. Currently, Deepak is beginning computational experimentations that rely on the GALLAHAD package.

Yiqi Zhu has begun the study of successive Linear Programming algorithms for the solution of nonlinear programs. These techniques were developed in the sixties by the chemical process industries but have not resulted in successful general-purpose NLP software. However, they appear to be promising for the solution of very large-scale nonlinear optimization problems with a very large number of nonzeros and degrees of freedom. We envision the development of a trust region technique that is provably convergent and is successful for such problems, when implemented on top of a robust and efficient linear programming solver. During this summer, Yiqi has implemented a simple successive linear programming algorithm under the GAMS environment. He has successfully solved a small collection of twenty small test problems and is currently experimenting with the development of robust initialization strategies.

Panagiotis Vouzis and **Joe Elble** have begun computational experimentation with advanced computing architectures. For less than $3000, we purchased a standard computer to which we added to Graphics Processing Units (GPUs). The combined system has an output of 1.25 GFLOPS. Panagiotis has been experimenting with parallel implementations of algorithms for the solution of systems of equations. In particular, Pahagiotis has implemented Kaczmarz's row projection method (KACZ), one of the first iterative methods used for large nonsymmetric systems. We are finding that while parallelism of KACZ allows considerable CPU time reductions per iteration, it nonetheless increases the number of iterations for this algorithm. In addition, we are finding that developing sparse matrix implementations is more challenging than implementing successful dense matrix implementations. Panagiotis is currently working with Joe Elble on the implementation of variants of the KACZ algorithm as well as on the development of alternative algorithms and sparse matrix data structures that may result in improved GPU performance.

Joe Elble has also been working on the problem of binormalization of a given matrix. Binormalization improves the condition number of a matrix and is important in the context of solving systems of equations. The GPU implementation developed by Joe for the composite Jacobi binormalization algorithm was found to be up to six times faster than a corresponding CPU implementation. The GPU implementation achieves a high rate of parallelism, and clearly scales better in terms of the size of the matrix.

THRUST 2—APPLICATIONS OF OPTIMIZATION IN BIOLOGY, CHEMISTRY, ENGINEERING, AND MEDICINE

Protein Structural Alignment

Student:
   Shweta Shah (Ph.D. Student at CMU)

Aligning proteins based on their structural (3D) similarity is a fundamental problem in molecular biology with applications in many settings, including structure classification, database search, function prediction, and assessment of folding prediction methods. Structural alignment can be done via several methods, including contact map overlap (CMO) maximization that aligns proteins in a way that maximizes the number of common residue contacts. A former student, Wei Xie, developed a reduction-based exact algorithm for the CMO problem. Our approach solves CMO directly rather than after transformation to other combinatorial optimization problems. We exploit the mathematical structure of the problem in order to develop a number of efficient lower bounding, upper bounding, and reduction schemes. Computational experiments demonstrate that our algorithm runs significantly faster than existing exact algorithms and solves some hard CMO instances that were not solved in the past. In addition, the algorithm produces protein clusters that are in excellent agreement with the SCOP classification. An implementation of our algorithm is accessible as an on-line server at http://eudoxus.scs.uiuc.edu/cmos/cmos.html. This algorithm currently represents the state-of-the-art algorithm for the CMO problem.

Shweta Shah, who joined the group in November of 2007, has been working on improving Wei's algorithm for this problem. Her first task was to produce an improved on-line server implementing the

algorithm developed earlier by Wei Xie. This has been successfully completed and the server is now available through archimedes.cheme.cmu.edu and provides external testing of the code. Her second task has been the development of heuristics for obtaining good solutions at the root node of the branch and bound algorithm that we have developed for this problem. Shweta's computations indicate that our dynamic programming-based bounds can be improved significantly by a randomized greedy heuristic, as well as a heuristic that exploits the presence of specific motifs in the protein structures to be aligned.

Protein-Ligand Docking

Student:　　　**Saurabh Awasthi (M.S. student at CMU)**
Collaborator:　**Professor Mike Domach (Chemical Engineering, CMU)**

A central problem in drug design is to identify small molecules that can bind on certain active sites of a protein and deactivate the corresponding function of the protein. Key to solving this problem is the ability to identify the site on a given protein where a given molecule is most likely to bind. This is frequently accomplished through the minimization of binding free energy. **Saurabh Awasthi**, who joined the group in November 2007, has been working on this problem. Saurabh has used the software package Autodock to provide binding energies for protein-ligand complexes from the protein data bank. He also utilized 14 of the derivative-free optimization solvers used in the work of Luis Miguel Rios (reported) above to find optimal docking positions. He has found that solutions provided by Autodock are not locally optimized and that the derivative-free solvers are able to provide improved (smaller) binding energies.

Design of Novel, Environmentally Benign Chemicals

Students:
　　　　Apurva Samurda (M.S. student at CMU)

Due to concerns regarding the depletion of the ozone layer by chlorofluorocarbon (CFC) refrigerants, extensive research efforts have been directed towards finding environmentally benign CFC replacements. In the mid 1980s, it was proposed that the search for appropriate Freon and other CFC replacements can be approached computationally by using group contribution techniques to predict properties of potentially new compounds. The main question is then how to efficiently search the astronomically large space of all potential group combinations in order to identify the most promising refrigerants.

In work funded by an NSF/Lucent Technologies Industrial Ecology Fellowship, we developed an optimization model and a systematic solution methodology for the Freon replacement search problem. Methyl chloride and other CFCs used as refrigerants in the past turned out to be some of the solutions of our model. Furthermore, our model was able to identify several *novel* potential alternative refrigerants (compounds that do not appear in chemical databases as well as some that appear but have never been used as refrigerants.) This is the first theoretical approach to propose novel potential refrigerants after finding the *complete* set of solutions to a Freon replacement problem that was open for the last 20 years.

Recently, we extended our approach to the problem of identifying replacements for refrigerants currently used in retail food refrigeration. With funding from the Environmental Protection Agency and the National Science Foundation, we identified over 3000 potential new secondary refrigerants. A paper on this subject is nearing completion. We currently plan to seek to hire a synthetic chemist as a postdoc in order to synthesize and test a carefully select subset of 12 of these compounds.

In the long term, we plan to develop similar computational and experimental techniques for the design of fire suppressants, industrial solvents, polymers, drilling fluids, and drugs with an emphasis on minimizing the environmental impact over the entire life cycle of the new compounds.

Apurva Samurda, who joined the group in November 2007, has been studying the problem of designing secondary refrigerants. He first used the model developed earlier by Nanda and Sahinidis in order to

identify potential new secondary refrigerants. Over 800 new potential refrigerants were identified using an efficient explicit enumeration approach. Many of them appear to be easily synthesizable and energetically more efficient than existing refrigerants. The enumeration approach requires running times that increase exponentially in the size of the designed molecule. For this reason, Apurva developed a novel model that relies on mostly linear group contribution techniques. Then, he used the linear portion of this model to find all solutions of the underlying MILP formulation with BARON. These solutions were subsequently screened using the nonlinear property prediction techniques as a filter. This has allowed Apurva to find many additional potential refrigerants that also appear environmentally benign and energetically efficient.

Erik Ydstie's Group

Adaptive Control Systems

New developments: **Submission of manuscript on robust adaptive control, Software for passivity based adaptive control. Methodology for multi-input single output adaptive control systems.**

Students: **Eduardo J. Dozal-Mejorada (Ph.D. May, 2008, now at Shell Global Solutions)**
Richard Chan (Post Doc researcher and ILS)
Keyu Li (PostDoc researcher and ILS)

Wayo (Eduardo) Dozal defended his thesis in May. In his thesis he developed theory and application of a novel approach for supervised adaptive control. He was able to develop a new approach for stability analysis of adaptive systems and he showed parameter convergence without knowledge of an upperbound of the disturbances. This is a new result and the paper has been submitted for review in Automatica. He also developed a convergence result for the least squares based adaptive controller which highlights robustness issues. This paper will be submitted for publication in the IEEE Transaction on Control. The supervision method can be applied for an online optimization technique for unconstrained optimization based on extremum seeking control. The optimization algorithm behaves as a stand-alone module using existing process models to gather information and adaptively drives the process to its extremum without altering the simulation code. The optimizer uses a second order approximation to a high order system and takes a set of modified equality constraints constructed so that they have the same geometric characteristics of the true steady-state behavior of the process. The module employs a dynamic model to obtain a steady-state model of the system. The steady-state model is then used to find the optimal input to the process. The optimum point obtained by the optimizer is tracked throughout process operation. The advantages of this adaptive algorithm over other traditional optimization approaches include: 1) it uses current process models, 2) it can handle multiple objective functions, 3) it only applies a subset of all process states, 4) it self-learning, and, 5) it is appropriate for steady-state or dynamic models. We have developed theoretical convergence and stability results for the exact-matching case and have started working on the robustness problem. Successful implementation has been applied to two case studies: 1) optimization of biomass production in a bioreactor, and, 2) optimization of silicon production in a reactor. Richard Chan has developed software implementations of multi-input single output predictive control systems for applications in the process industries. The user interface is in the final stages of development and the algorithms will be ready for industrial testing in 2009. Keyu Li has developed a software solution for passivity based adaptive control. The algorithm has been tested in simulation on an ethylene cracking process and a selective catalytic reactor for NOX reduction in coal fired power plans. The software can be interfaced with standard DCS using the Microsoft OPC interface.

Passivity Based Modeling and Control

New developments: **New stability results for the reactive, multi-component flash**

Students: **Yuan Xu (Ph.D. June, 2008, now at OSI Soft)**
Mohit Aggarwal (Ph.D. expected 2009)

Yuan has developed results that demonstrate uniqueness and stability of the multi-component-multi-phase flash. He extended these results to the reactive flash. The key to understand the problem came from a re-reading of Gibbs old papers and the application of some new geometric results concerning the degree of smoothness of convex hulls of multiple continuous functions. Yuan is in the process of writing up several papers describing the progress made in this very classical area of chemical engineering analysis. The focus of this research has now shifted to passivity-based control of multiphase systems with reaction transport (diffusion and convection) and the design of asymptotic observers. Proportional control is currently being used to explore the controllability, stability, and sensitivity of the system. However we plan to extend the result to more complex control algorithm and model predictive control. Mohit has started the development of stability theory for systems with time-varying reference. This class of systems is referred to as contracting systems and the theory has application distributed, web-based simulation and control. Mohit has worked on modeling chemical process systems using invariant groups, He has made good progress in the development of reduced order models using process invariants for the gasifier in the IGCC process and the carbothermic aluminum process.

Carbothermic Aluminum Production

New developments: **Paper submitted on modeling and control of the VRR**

Students: **Yuan Xu (Ph.D. June, 2008, now at OSI Soft)**
Mohit Aggarwal (Ph.D. expected 2009)
Balaji Sukumar (PostDoc researcher)

Carbothermic reduction takes carbon and aluminum oxide feed to produce aluminum. Work thus far has included developing a model using MATLAB to describe a variation of this process, as is being created by ALCOA, the world's largest aluminum producer. Yuan Xu developed an interface between the ChemApp/FACT thermodynamics program with MATLAB via a MEX Interface. This program allows the model to handle ranges of temperatures and compositions without extra work needed to determine equilibrium constants, activity coefficients, and extent of reactions. Another improvement has been to incorporate computational blocks using the SIMULINK tools in MATLAB and an interface with COMSOL CFD code. Not only will this give the model a more "user-friendly" interface, but it will also allow for the exploration of modular simulation, where numerous monolithic simulation blocks can be combined and individually interchanged or altered without major recoding needed to modify the overall model. The vapor recovery section of the carbothermic aluminum process has been modeled. The primary reaction in the column, the gas flows as well as solid transport. The focus is to develop efficient methods to represent the thermodynamics and the multiphase behavior of the VRR. Mohit has developed a three phase (liquid/solid/gas) multi-scale, simulation model which will be used for system design, scale-up, economic evaluation and control studies. A variety of models have been developed for primary reactor under steady and cyclic operating conditions. Balaji has developed simulation models and control system structures for the entire process. He is now in the process of developing micro-models for studying dust formation and condensation which will help in the control of the reactor process.

Process Networks with Application to Energy Problems

New developments: **Software has been developed for simulation of coal fired power plants**

Students: **Michael Wartman (Ph.D. expected 2010)**
Chengtao Wen (PostDoc Researcher)
Kendell Jillson (Ph.D. 2007, PostDoc researcher)

Michael developed a process analog of the Tellegen theorem of electrical network theory. He introduced a novel modeling framework for studying dynamics, distributed control, and optimization of complex chemical process networks. We are interested in developing distributed control systems that self-organize

so that stability and optimality follows as a consequence of how the networks are put together and how they are connected with boundary conditions or other networks. By considering only the topology of the system, basic conservation principles and the second law of thermodynamics we have developed a multi-component analog to Tellegen's Theorem of electrical circuit theory. This result has been combined with the passivity theory of nonlinear control. It is shown that under certain convexity conditions the network converges to a stationary solution. Under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized. Kendell Jillson has used the theory to develop control system structures for the IGCC process. He has shown that passivity based control systems can be used to stabilize and control the IGCC. Chengtao Wen has been involved with a modeling team at Emerson process management which has implemented models and developed suing the thermodynamic theory into a complete system for design and evaluation of process control systems in coal fired power plants. Chengtao and Michael are now working on synchronization problems. The idea here is that that the models need to synchronized with on-line data in real time. Chengtao is working on synchronization in the power industry whereas Michael is working synchronization in oil and gas field production

Multi-Scale Modeling of Particulate Processes with Fluid Flow

Student: Juan Du (Ph.D. expected 2010)

This research addresses modeling and control of yield and size distribution in particulate processes. We use a novel method for solar-grade silicon production, the thermal decomposition of silane gas in a fluidized bed reactor, as a benchmark. We have developed a model and control scheme for the behavior of particles in a fluidized bed reactor based on silicon production. The model simulates growth of silicon particles with ordinary differential and algebraic equations that track particle movement through discrete size intervals. The model solves quickly and is easily tuned to fit experimental data. The passivity-based inventory controller maintains a constant mass of a specified size of silicon particles. The results from this research will be published in Powder Technology.

Last year we have matched the model to pilot-scale process data obtained from Solar Grade Silicon LLC in Moses Lake, Washington. We developed an observer for on-line estimation of process states and parameters. The method allows for estimation of particle size distribution in real time. We have combined the observer based modeling scheme with inventory control for total mass and seed-mass control for on-line stabilization of the particle size distribution. The model and control scheme is being used for scale-up and control system design for production system under current development at SGS. It expected that that when the new process is in operation that it will provide several competitive advantages relative to the current Siemens process, including higher throughput per process unit, lower capital cost and significantly lower energy usage.

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