CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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ANNUAL REVIEW MEETING

Please take note that the next **Annual Review Meeting** will take place on **March 9-10, 2009**. This will be followed by the meeting of the special group on **Enterprise-wide Optimization on March 11**. We will hold a reception on Sunday, March 8, in the new renovated 4th floor of Doherty Hall, next to the new **CAPD Conference Room**. The first day of the meeting, Monday, March 9, will consist of overviews given by Larry, Ignacio, Nick and Erik, followed by a discussion with industrial participants, and a poster session by the students. As we did last year, we will host a group dinner that evening at Monterey Bay Fish Grotto Restaurant. The second day, Tuesday, March 10 is devoted to final year student presentations. In the afternoon, 1:30 to 4:30 PM, there will be a special session on **Stochastic Programming** that will include a tutorial on formulations, computational methods and modeling tools. The speakers will be **Prof. Jeff Linderoth** from Wisconsin, and representatives from **GAMS** and **AIMMS**. This session is actually part of the Enterprise-wide Optimization project (see next section), but will be open to all CAPD members as we did last year.

The detailed agenda of the meeting will be sent very soon. Also, if you are interested in giving a short presentation, please let us know. We promise that we will give more time than we did last year. Also, if you have any suggestions for the format of the meeting, please let us know.

ENTERPRISE-WIDE OPTIMIZATION

The meeting of the EWO group took place on September 30. The group is currently composed of the following companies: ABB, Air Products, BP, Dow Chemical, ExxonMobil, NOVA Chemicals, PPG, Petrobras, Praxair and Total. These companies have supplied case studies that are being undertaken by the EWO faculty and students. The project involves a total of 7 Ph.D. students, and 5 faculty (CMU: Larry Biegler, Ignacio Grossmann, John Hooker; Lehigh: Larry Snyder; UPitt: Andrew Schaeffer,). As indicated above, the EWO meeting will start on Tuesday, March 10 at 1:30 PM with the special session on Stochastic Programming for Enterprise-wide Optimization, and continue on Wednesday, March 11, 9:00 AM to 2:30 PM, focusing on reporting the current projects. Companies who might be interested in joining this group in fiscal year 2009, please contact Ignacio Grossmann. The membership fee to this group is $12,500 for members of the CAPD. A description of the EWO project can be found in http://egon.cheme.cmu.edu/ewocp/

The Special Issue on Enterprise-wide Optimization (EWO) in *Computers & Chemical Engineering* edited by Kevin Furman and Ignacio Grossmann was published as Volume 32, Issue 11, pp. 2479-2838 (24 November 2008). The issue involves a total of 20 papers, with 4 of them from industrial authors (Air Products, Dow Chemical, ExxonMobil, Honeywell). The first ten papers deal with supply chain issues. The next set of four papers deal with solution approaches to scheduling problems, and the last four papers focus on operational issues.

CAPD SHORT COURSE

- As an experiment we will offer our new **CAPD Short Course** immediately following the CAPD Annual Meeting: http://capd.cheme.cmu.edu/shortcourse/index.html. The CAPD Short Course will take place on March 12-18, 2009. The course, **Optimization Modeling and Integrated Process Operations** is organized in two parts consisting of 6 modules which can be taken in any combination (e.g. 1, 2, 3 or all 6):

I. Optimization Modeling to be taught from Thursday through Saturday (March 12-14) will focus on modeling and algorithms with applications to process optimization, process synthesis and molecular design:

   a) Nonlinear programming (Biegler, Thursday, March 12)
   b) Mixed integer and disjunctive programming (Grossmann, Friday, March 13)
   c) Global optimization and optimization under uncertainty (Sahinidis, Saturday, March 14)

II. Integrated Process Operations to be taught from Monday through Wednesday (March 16-18) will focus on three major decision levels in plant and enterprise-wide optimization:

d) Mixed-integer models for planning and scheduling (Grossmann, Monday, March 16)
e) Integrating computation, communication and control in complex process networks (Ydstie, Tuesday, March 17)
f) Differential/algebraic models for real time optimization (Biegler, Wednesday, March 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. Recall that CAPD members receive a 25% discount. 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.

GENERAL NEWS

The CAPD Newsletters can now be accessed thorough the webpage http://capd.cheme.cmu.edu/newsletters.html. All registered users of CAPD can access these by using their email addresses as userid and password. We also welcome any suggestions you may have for our webpage http://capd.cheme.cmu.edu

CAPD Conference Room
As part of the laboratory renovations of the Department of Chemical Engineering in Doherty Hall, we are pleased to inform you that the CAPD now has its own conference room. It is located in DH4201 (CAPD Conference Room). Also, there is a new elevator that takes you directly to the 4th floor. The area next to the elevator on the 4th floor has a very nice view of the campus, and that is where we will hold our reception on Sunday, March 8, 7:00-10:00PM. As part of the renovation project, students on the 4th floor (about one half of the total) have nice new cubicles with AC. Unfortunately, the students on the 3rd floor will have to wait for the next round of renovations to get similar facilities.

AIChE Meeting. The four faculty of the CAPD gave a total of 34 presentations at the Annual AIChE Meeting in Philadelphia, November 17-21, 2008. These are listed in the CAPD e-Newsletter that we sent on November 4, 2008.

Larry Biegler gave an invited talk on "Large-scale Nonlinear Programming for On-line Optimization" as part of MIT's Computational Design and Optimization Distinguished Speaker Series. At the November AIChE meeting he presented a special talk on Dynamic Real-time Optimization. In December, he presented a seminar on "Dynamic Real-time Optimization: Reconciling Rigorous Models and Fast Computation" at the Universidad Iberoamericana. This summer Larry will spend a month as a visiting professor at Zhejiang University, Hangzhou, China. Finally, Larry has been offered the Hougen Visiting Professorship at the University of Wisconsin and will spend part of Fall, 2009 in Madison, WI.

Ignacio Grossmann was named one of the "One Hundred Engineers of the Modern Era", http://www.aiche.org/uploadedFiles/About/Centennial/100modernerachemeng.pdf by AIChE. He was recognized for his work on MINLP for design and operations. Ignacio delivered the plenary lecture "Optimization Models and Strategies for Crude Oil Operations and Offshore Oil and Gas Production," at the CLAIO-2008 Meeting (Latin American Congress of Operations Research), in Cartagena, Colombia. He also delivered the plenary lecture "New Research Trends in Process Systems Engineering: Product and Process Design, Energy and Sustainability, Enterprise-wide Optimization," at the 11th Mediterranean Congress of Chemical Engineering, Barcelona (2008). Ignacio gave two special talks at the AIChE Meeting: one on Process Synthesis and Optimization at George Stephanopoulos's session, and the other on the role of math programming in planning and scheduling. Ignacio also delivered the lecture "Generalized Disjunctive Programming: A Framework for Formulation and Alternative Algorithms for MINLP

Optimization," at the IMA workshop on MINLP: Algorithmic Advances and Applications. You can watch his lecture in http://www.ima.umn.edu/videos/?id=642. Ignacio gave a short course on Enterprise-wide Optimization at PPG, and participated in the advisory board meetings of the Department of Chemical Engineering at Cornell University, 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 gave a plenary talk on "Challenges in biological informatics" at the 100th Annual Meeting of the American Institute of Chemical Engineers, Philadelphia, Pennsylvania, November 2008. At the INFORMS meeting this past October, Nick organized the *Bioinformatics and systems biology* cluster with five invited sessions. This semester, Nick graduated his first four MS students. His group currently includes 15 students, postdoctoral researchers, and visitors. The special issue he is editing on global optimization for the journal *Optimization Methods and Software* is now nearing completion and will include at least 19 papers. Nick is currently serving on the scientific program committees of the following conferences: (1) The 6th International Conference on Integration of AI and OR Techniques in Constraint Programming for Combinatorial Optimization Problems, Pittsburgh, PA, May 2009; (2) Computational Management Science, Geneva, Switzerland, May 2009; (3) Foundations of Systems Biology in Engineering (FOSBE 2009), Denver, Colorado, August 2009; (4) Foundations of Computer Aided Process Design 2009 (FOCAPD 2009), Breckenridge, Colorado, June 2009. Along with Chris Floudas, he is co-organizing the global optimization cluster for the 2009 International Mathematical Programming Symposium, Chicago, Illinois, August 2009.

Erik Ydstie took leave of absence to write an undergraduate textbook on process control and lead iLS Inc. He completed about 300 pages using the ideas from his research on passivity based and inventory control. The material will be used in the process control class in 2009. The Laplace transform is eliminated and nonlinear systems are discussed along with linear systems. Optimization based methods are included to deal with batch process control system. Erik also worked as CEO of iLS. iLS has currently 4 full time and 4 part time employees. The adaptive PID and process identification products are near completion. The company is developing a large scale adaptive MPC product with "configuration-on-the-fly" capabilities. Erik presented a three day short course on adaptive control at NTNU in Trondheim for Diploma Engineering Students. He took part in a due diligence process for a large solar grade silicon investment and continued technical consulting with Alcoa and PPG

Congratulations to **Christos Maravelias**, former student of Ignacio, and current faculty member at the University of Wisconsin-Madison, who received the 2008 W. David Smith, Jr. Graduate Student Paper Award given by the CAST Division of AIChE. The award is for his paper, "Simultaneous Planning for New Product Development and Batch Manufacturing Facilities," published in *I&EC Research* 40, 6147-6164 (2001).

Congratulations to **Victor Zavala**, who joined Argonne National Laboratory as a postdoctoral research fellow. Victor has accepted a faculty position in the Chemical Engineering Department at the University of Texas. Welcome back to **Rodrigo Lopez Negrete** who completed an internship at Pfizer in the fall semester.

Congratulations to **Bora Tarhan** and **Fengqi You**, students of Ignacio, for having won CHEGSA Symposium awards for their presentations. Congratulations also to **Ravi Kamath**, student of Ignacio and Larry, for receiving an honorable mention award. Congratulations to **Michael Wartmann** and **Fengqi You** who were selected to receive a travel grant from CAST in conjunction with the AIChE meeting in Philadelphia.

Congratulations to **Michael Wartmann,** student of Erik, **Weiji-Lin** student of Larry**, Sreeram Vetukuti,** student of Larry, **Ravi Kamath**, student of Ignacio and Larry, and **Juan Pablo Ruiz**, student of Ignacio, for having passed their Ph.D. proposal exam

Congratulations to **Deepak Channamariyappa** for completing his M.S. thesis on *Preprocessing in Linear Programming.* Deepak is staying as a visiting researcher in Nick Sahinidis' group. Congratulations to

Xuan Shi for completing his M.S. thesis on *Deterministic Global Optimization in Neural Network Training.* Xuan is staying as a visiting researcher in Nick Sahinidis' group. Congratulations to **Yiqi Zhu** for completing his M.S. thesis on *Computational Implementation of a Successive Linear Programming Algorithm.* Congratulations to **Saurabh Awasthi** for completing his M.S. thesis on *Molecular Docking by Derivative-free Optimization Solvers.* Saurabh has joined Kinapse Information Processing and Consulting, Philadelphia, Pennsylvania.

Congratulations to **Apurva Samudra**, **Shweta Shah**, and **Keith Zorn**, who passed their Ph.D. qualifying exam.

Congratulations to **Harshad Godke** of Erik Ydstie's group who graduated with a Master. He will work on a Ph.D. in Bio-Physics.

Congratulations to **Siddarth Raman** of Erik Ydstie's group who graduated with a Master. He will join Merck Company.

It is a pleasure to welcome the following new students to the PSE group. **Robert Smith** (Florida State University) who will work with Larry and Myung Jhon in the area of fuel cells. **Vijay Gupta** (IIT Roorkee) who will work with Ignacio in the area of oil and gas field exploration under uncertainty. The following new students joined Nick's group: **Chris Cleveland** (from University of St. Thomas), **Yan Zhang** (from Zhejiang University, China), **Danan Wicaksono** (BS from Institut Teknologi Banduny, Indonesia; MS from National University of Singapore), **Satyajith Amaran** (from National Institute of Technology Karnataka, India), and **Rohan Desai** (from Dwarkadas J Sanghvi College of Engineering, India). Chris and Yan are Ph.D. students and will work on different aspects of risk assessment in CO2 sequestration. The other three students are M.S. students and will work on parameter estimation (Satyajith), protein-ligand docking (Danan), and portfolio optimization (Rohan).

Dr. Pedro Castro from INETI, who worked on a project on batch scheduling with ABB, and **Elisabet Capon**, Ph.D. student from Dr. Puigjaner's group in Barcelona (UPC), who worked on a supply chain project for Praxair, have returned to their countries. **Dr. Edwin Zondervan** from the PSE group at Eindhoven and **Dr. Mariano Martin** from Salamanca, Spain, will join Ignacio's group later in the spring.

CAPD e-News. We sent on November 4 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 which 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.

UPDATED VIRTUAL LIBRARY ON PROCESS SYSTEMS ENGINEERING

You may want to learn about an update of the virtual library on Process Systems Engineering, http://cepac.cheme.cmu.edu/pasilectures.htm This library was initially created from the workshop Pan American Advanced Studies Institute (PASI-2005) on Process Systems Engineering that took place on August 16-25, 2005, in Iguazú, Argentina. The library has been updated with material from the second workshop PASI-2008 on Emerging Trends in Process Systems Engineering that took place in Mar del Plata, Argentina, August 12-21, 2008. The goal of both these workshops was to provide a state-of-the-art review and to bring together faculty and Ph.D. students from various countries in the Americas (U.S., Canada, Mexico, Argentina, Brazil, Chile, Colombia and Venezuela).

The PASI-2005 workshop covered the following areas:
- Optimization, Process and Product Design, Process and Supply Chain Operations, Process Dynamics and Control, and material on these topics can be found in:
http://cepac.cheme.cmu.edu/pasi2005/slides/index.htm
while the PASI-2008 covered these areas: Advanced Modeling Tools, Biosystems Engineering, Multiscale Design of New Materials, Complex Engineering Systems, Sustainability, New Energy Systems, Enterprise-wide Optimization. Material on these topics can be found in:

http://cepac.cheme.cmu.edu/pasi2008/slides/index.html

The virtual library, http://cepac.cheme.cmu.edu/pasilectures.htm , consists of the Powerpoint slides of the presentations of each topic, which are largely tutorial in nature. These are complemented with background articles that provide comprehensive reviews. Exercises, as well as MATLAB and GAMS files are also available, including comprehensive exams for each workshop that contain questions with answers. Members of the CAPD should find the material to be helpful since it contains useful overviews of areas that are of current interest and that are not normally found in textbooks and reference texts. We intend to periodically update the presentations, and we would appreciate your feedback or comments.

WEBSITES/PROCESS SYSTEMS DIRECTORY

In addition to the Virtual Library on PSE, 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 and improved at IBM. These have seen a number of applications ranging from detailed fuel cell models, advanced gas adsorption 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. The components of this work are detailed in three reprints listed below. 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 to three 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 a wide variety of NLP problems. This approach is not restricted to particular NLP solvers. The general framework is described in a reprint listed below. Moreover, this approach has been demonstrated on a variety of process control and dynamic applications. A preprint that describes this approach is also 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 in the preprint listed 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 approaches 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 completed a new solution approach for the global optimization of Bilinear and Concave 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**, and **Jon Lee and Andreas Waechter at IBM,** the NSF project on Cyberinfrastucture for MINLP has produced five problems, and specifications for the architecture of the website which is under construction. Testing on the open source code *Couenne* for the global optimization of MINLP problems continues. **Aldo Vecchietti** has updated the website for LOGMIP http://www.logmip.ceride.gov.ar/ which is now available in GAMS (http://www.gams.com/dd/docs/solvers/logmip.pdf).

Ravi Kamath has completed a novel mathematical model for multistream heat exchangers and a group method for the simulation and optimization of distillation columns. **Jose Caballero's** manuscript on kirging models for the optimization of process flowsheets has been accepted for publication. **Elvis Ahmetovic** has started a new project on water management in biofuel plants. **Gonzalo Guillen** completed a manuscript on a bi-criterion optimization approach for the design and planning of hydrogen supply chains for vehicle use.

Bora Tarhan has completed a manuscript for the optimization of oilfields with nonlinear reservoir models, and has developed a hybrid strategy where valid bounds can be obtained with outer-approximation iterations and two global optimization calculations. **Sebastian Terrazas** has developed in collaboration with Dow a novel MILP model for optimizing the availability of process networks with uncertain demands and process availabilities in which capacity expansions and intermediate storage tanks are considered. **Fengqi You** has completed a new paper on integrated multi-echelon supply chain design with inventories under uncertainty for which he has formulated new MINLP models. He also is completing a new manuscript in collaboration with Pedro Castro on Dinkelbach's algorithm for linear fractional MINLPs. Also, in collaboration with Elisabet Capon and Praxair, he has developed several strategies for vehicle routing and tank-sizing. **Sylvain Mouret** has completed the manuscript on a priority slot for crude oil scheduling in which he implemented novel symmetry breaking constraints that produce large computational savings. He is also developing interesting generalizations for scheduling models (single-operation and multiple-operation sequencing). **Abdul Attalas** is completing a novel aggregated CDU model that can explicitly handle steam stripping and has the capability of predicting inverted temperature profiles. **Ricardo Lima** is developing a scheduling model for PPG for the production of tinted glasses. **Roger Rocha**, a postdoctoral fellow from PETROBAS, has completed a manuscript on computational strategies for a petroleum allocation obtaining very significant savings mathematical Model and A Solution Algorithm, manuscript on tested disjunctive decomposition technique for petroleum large scale supply chain problems. **Pedro Castro** completed a manuscript in collaboration with ABB on discrete and continuous time scheduling formulation for continuous plants under variable electricity cost. Finally, **Rosanna Franco** has completed the 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/

Nick Sahinidis' Group

There have been a number of major new developments from Nick Sahinidis' group since the previous newsletter.

1. In global optimization, **Xiaowei Bao** has completed a computational experimentation with multiterm, as opposed to single term, relaxations for quadratic constraints and found that these relaxations expedite BARON significantly for the solution of quadratically constrained quadratic programs. A related paper has been submitted to *Optimization Methods and Software*.
2. In the area of global MINLP optimization, Nick has completed a preliminary implementation of MIP relaxations with BARON. These relaxations are currently solvable only with the Xpress MIP code, but we plan to make them available with the Cplex MIP code as well. A related paper was presented at INFORMS and demonstrated that nearly twice as many MINLPs from IBMLib can now be solved to global optimality, compared to BARON's previous LP relaxations.
3. **Yiqi Zhu** has developed a preliminary implementation of a successive linear programming solver. The solver was applied to many quadratic and general nonlinear programs, successfully solving nearly all problems it was applied to.
4. **Joe Elble** and **Panos Vouzis** have developed a parallel implementation of iterative linear equation solvers on Graphics Processing Units (GPUs). A related paper was submitted to *Parallel Computing* and demonstrates that a GPU/CPU combination (for a cost less than 3K) outperforms a cluster of 16 Linux workstations.
5. New formulations and results for quantum chemical calculations using a high-order RLT reformulation **(Keith Zorn)** structural alignment of proteins using a problem-specific heuristic **(Shweta Shah)** and molecular design using a linear reformulation of the problem **(Apurva Samudra)**.

Erik Ydstie's Group focuses on process modeling, nonlinear and adaptive control. In the area of adaptive control, we have been working on developing a new approach to adaptive PID control which is based on global optimization and frequency domain specifications for the closed loop performance. The controller has been tested in simulation studies. Experimental studies are planned for the spring of 2009 in the pilot plant in the Rothfus lab. These experiments will be carried out by a new master student. **Juan Du** has continued the work on nonlinear control theory. She developed a continuous time version of the switching lemma developed by Wayo in his last year at CMU. She is now starting to work on a new line of research for nonlinear control using results based on the idea of converging systems. **Michael Wartmann** has been at the Shell research labs in Delft working self-optimizing control of oil fields. He has developed some new optimization principles based on the Tellegen theorem which appear to have very broad applicability. **Mohit Aggarwal** completed his work on modeling bio-gasification processes. This work was carried in cooperation with Kevin Fuhrman at Air Products. He also made good progress on developing stability results for reactive flash systems with applications to modeling the gasification systems and the Alcoa carbothermic reactor system. Rooco Panella joined the research group. He will be working on developing flexible, dye sensitized solar cells. Manfred Morari edited the CAST lecture Erik gave at the AIChE meeting in Salt Lake City. The mvie can be found at the following link (big file): (http://control.ee.ethz.ch/%7Emorari/download/CAST%202007_Ydstie.mov). **Keyu Li** has developed a new approach for adaptive PID control with feedforward from measured disturbances. **Chengtao Wen** has developed distributed, dynamic simulation models for coal fired power plants. The approach for distributed dynamic simulation is based on the method developed by Vianey in her Ph.D. with Erik in 2004. The method is based on the use of asynchronous recording controllers which record and control the simulation error.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: **Victor M. Zavala (Ph.D. completed Fall, 2008)**
Visitor: **Kexin Wang, Zhejiang University (PhD completed Fall, 2008)**

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 with up to millions of variables could be solved in only a few CPU minutes. More recently, this approach has been extended, by using either a Schur complement strategy for multi-scenario problems or advanced sparse decomposition strategies for general problems. Using an efficient pre-processing step, small subproblems can be derived and design scenarios can be identified more precisely and efficiently. This approach is described in the reprints 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 reprint 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 has been 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.

A number of reprints that describe these features, and co-authored by Carl and Victor, are listed below. Moreover, Victor has recently presented the application of this work to large-scale polymerization process operation at the November AIChE meeting.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: Brian Baumrucker (Ph.D. started Fall, 2004)
Krishna Iyengar (MS started Fall, 2008)

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.

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; it has also enjoyed widespread use in projects with the McMaster University. 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.

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 and real-time optimization formulations with switching variables. A general framework that describes the MPEC formulation for these problems is described in a reprint listed below.

More recently, Brian has extended this approach to dynamic optimization problems, where switching conditions can occur at any point in time. This class of hybrid dynamic systems provides an interesting challenge; it can lead to very large MINLP problems but can be treated in a straightforward way using MPEC strategies. The preprint listed below provides a detailed description of this approach along with a demonstration of their performance on two hybrid dynamic optimization problems. On one problem, dealing with the optimal trajectory of a racing car, results were obtained that represented significant improvements over literature values. Finally, Brian has adapted this approach to 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 can solve very large optimization problems (with the equivalent of many thousands of switching variables) within only a few CPU minutes. This allows the optimal exploitation of inventory in pipelines in order to reduce energy and other operating costs, while still meeting customer demands. The results of this work were presented at November AIChE meeting. A preprint of this study will appear in the next newsletter. **Krishna Iyengar**

will continue this pipeline scheduling study through the consideration of a number of multi-period scenarios.

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. 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://ww.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 three reprints below.

Weijie Lin recently passed her Ph.D. proposal exam. She 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 also investigated optimal control strategies that improve the product quality and reduce production time. Preliminary results indicate significant performance gains (around 15%) can be obtained with quite different, novel operating strategies for operation of the polymer process. This work was presented at the November AIChE meeting and will appear as a preprint in the next newsletter.

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 was a featured presentation at the 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. This work was also presented at the November AIChE meeting.

Finally, **Rodrigo Lopez Negrete** is extending this model-based control approach to stochastic processes with uncertainties in states and outputs. This work benefits from a collaboration with **Prof. Sachin Patwardhan** at IIT-Bombay, an expert on nonlinear control and identification. Currently, Rodrigo has adapted recently developed Unscented Kalman Filter (UKF) methods, which deal with non-normal noise structures, to the MHE formulation described above. In recent tests, Rodrigo has shown that this strategy has superior performance to Kalman Filter approaches as well as previous MHE strategies. Working with

Prof. Patwardhan, Rodrigo continues to refine this approach and also is also extending this MHE strategy to incorporate recently developed particle filter and ensemble filter strategies.

Large-Scale Optimization for Fuel Cell Models

Researchers: Parag Jain (Ph.D. started Fall, 2005, joint with Prof. M. S. Jhon)
Robert Smith (Ph.D. started Fall, 2008, 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 this reprint, 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. Finally, Parag has extended this approach to fully 3D models of the integrated MEA and its coupling with the gas channel. This work was presented at the November AIChE meeting. Parag's current work is to extend these concepts to molecular dynamics models to improve the water and proton transport properties of the polymer membrane. **Robert Smith** has recently joined the group and will continue this direction on the project.

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** just passed his PhD proposal. In this work, he 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 was presented at the November 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)
Jyoti Swankar (MS started Fall, 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 are IGCC-based coal-fired power plants that include 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. This work is described in the preprint listed below. The work on reduced order modeling and optimization will be extended to further 3D PDE applications through the MS work of **Jyoti Swankar.**

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. This work was presented at the November AIChE meeting. A preprint of this work will appear in the next newsletter.

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. proposal 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 is hardly any simulation or optimization based process models for MHEX available in the open literature which takes 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 (as described in the MPEC project above). 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. Both of these projects were presented at the November AIChE meeting. Preprints of this work will appear in the next newsletter.

Ignacio Grossmann's Group

Cyberinfrastructure for MINLP Optimization

New developments: **Five problems for MINLP library and design of architecture of website**

Student: **Juan Pablo Ruiz [started Jan 2007]**
Collaborators: **Larry Biegler, Nick Sahinidis, Francois Margot, Pietro Belotti (Lehigh)**

With funding from NSF we are creating 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 have developed five new MINLP optimization problems: a) Supply chain inventory problem (You, Grossmann), b) Water treatment network (Ruiz, Grossmann), c) MPEC formulation for some discrete constraints (Baumrucker, Biegler), d) X-Ray diffraction (Smith, Sahinidis), e) Cyclic scheduling (Castro).

We have also established the architecture of the website to allow for multiple authors to submit alternative formulations or instances for any given problem. The website is under construction and should be available later in the spring.

Pietro Belotti, who has been developing *Couenne* an open-source code for solving nonconvex NLP and MINLP problems, has moved to Lehigh as a Visiting Assistant Professor. 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. Pietro has written the code CouenneSolverInterface that allows the implementation of various bound tightening techniques, and branching strategies. Last few months have concentrated on extensive testing of branching decisions. We should note that *Couenne* is available in the COIN-OR library: http://www.coin-or.org/projects/Couenne.xml

Algorithms for Nonlinear Disjunctive Programming

New Developments: **Redundancy for Strengthening Lower Bounds; New LOGMIP website**

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

Juan Ruiz

The project of Juan, who successfully passed his proposal exam, 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 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. Of course there are many options that are possible on how to perform the intersections. To address this issue 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.

Juan has applied the above procedure to 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 all these problems there were significant improvements in the lower bounds. This in turn led to a significant reduction in the number of nodes in three of these problems. Juan has almost completed this manuscript which will be submitted soon for publication.

In another interesting line of work Juan he has explored the idea of including redundant equations in the formulation in order to strengthen the lower bounds. The motivation comes from the fact that when nonconvex terms are replaced by convex envelopes this leads to a significant relaxation of the feasible region. This in turn means that constraints that are redundant in the original model may not be redundant in the relaxation. Typical case is in a process network when bilinearities in mixers are replaced by McCormick envelopes. In this case the total mass balance, originally a redundant constraint, becomes non-redundant in the relaxation and hence provides a cut. This work is still prelimary but Juan has tested this idea on 4 problems including 2 electric power networks, one process network and one batch process. The improvements in the lower bounds ranged between 36 and 93%.

Aldo Vecchietti: LOGMIP and DICOPT

Aldo has developed at INGAR 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. Aldo has updated the page for LOGMIP. See: http://www.logmip.ceride.gov.ar/

Optimal Synthesis of Integrated Gasification Combined Cycle (IGCC) Systems

New developments: **Models for multistream exchanger, group method for distillation columns**

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

Ravi successfully passed his Ph.D. proposal exam. This is a project in collaboration with Larry Biegler 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 achieve a higher thermal efficiency and to 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 has as an objective 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.

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. Ravi has 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 with specified temperature approaches. He has obtained very good results for the Shell, GE and ConocoPhilips entrained gasifiers. 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.

To address the superstructure optimization, Ravi has been developing a 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 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. Ravi has focussed 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, the 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 in optimization case studies where 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. Ravi has compared his model (3 integer variables, 300 variables and constraints) with the MINLP optimization model by Viswanathan and Grossmann (1993) (100 0-1 variables, 1500 variables and constraints) and found that he can solve the problem in only few seconds compared to over 20 minutes using SBB. While the number of trays and location of the feeds were in good agreement, the aggregate model tends to overestimate the loads in the reboiler and condenser by about 10%. Nevertheless, it is clear that the proposed model can be useful for preliminary calculations. Ravi is in the process of writing a paper on this work.

Ravi has also developed models for the multi-stream heat exchangers (MHEX). 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 developed a general nonlinear equation-oriented model for MHEX which is based on the pinch moel by Duran and Grossmann 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. The inlet and outlet temperatures of substreams are assigned appropriate values using a disjunctive representation involving Boolean variables 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 or as a continuous model by solving an inner minimization problem with complementarity constraints. 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. 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. Ravi's result (15.4 MW) compares favorably with previous work by Robin Smith (24.5 MW) and Sigurd Skogestad (17.4 MW). Ravi is in the process of writing a manuscript on this model.

Using these equation-oriented models, Ravi is also 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: Paper published on Flowsheet optimization using kirging model

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

Jose Caballero's recent work has been on incorporating process simulators for MINLP optimization in process flowsheets.

Jose's work has addressed the rigorous optimization of nonlinear programming problems in which the objective function and (or) some constraints are represented by 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 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 convergence cannot be guaranteed 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 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 has appeared recently in AIChE J. and is enclosed as a reprint.

Water Management Networks in Biofuel Plants

New development: Gathering literature information

Post-doctoral fellow: Elvis Ahmetovic (started September 15, 2008)

This is a new project by Elvis Ahmetovic in which he has been investigating the issue of water consumption in biofuel plants. He has especially concentrated in bioethanol plants for which he has gathered literature and data on water consumption, lost water in cooling towers and reuse in these plants. He has also used the mass and energy balance of the Cargill case study on bioethanol developed by Karuppiah and co-workers. Elvis is in the process of formulating a superstructure for water networks for reuse and treatment along the lines of Karuppiah's model. The objective is to minimize the consumption of freshwater in bioethanol plants, which in some cases is as high as 3 gals of freshwater/gal ethanol.

Design for Sustainability

New development: Bi-criterion optimization for hydrogen supply chains for vehicle use

Post-doctoral fellow: Gonzalo Guillen [University Roviri e Virgili, Tarragona]

Gonzalo 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 developed a model 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 has been 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 variability of the Eco-Indicator 99 under uncertainty is controlled by reducing the probability of exceeding a specified target level. Gonzalo formulated this problem as a bi-criterion MILP. 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 analytically obtained. 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, while 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. 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. The proposed decomposition strategy can provide the whole set of Pareto optimal solutions in a fraction of the CPU time required in the standard ε-constraint method. The manuscript on this work has just appeared in *AIChE J*. and is enclosed.

Gonzalo 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.

In recent work Gonzalo has addressed with Fernando Mele the design of hydrogen supply chains for vehicle use with economic and environmental concerns. The work is based on a case study considered by Almansoori and Shah (2006) in which they considered the cost of these supply chains. The problem is as follows. Given a set of available technologies to produce, store and deliver hydrogen, the problem consists of determining the optimal design of the production-distribution network capable of satisfying a specified hydrogen demand. The design task is formulated as a bi-criterion MILP, which simultaneously accounts for the minimization of cost and environmental impact. The environmental impact is measured through the contribution to climate change made by the hydrogen network operation. The emissions considered in the analysis are those associated with the entire life cycle of the process, and are quantified according to the principles of Life Cycle Assessment (LCA). To expedite the search of the Pareto solutions of the problem, Gonzalo used a bi-level algorithm in the spirit of Ramesh Iyer's work. The main result that emerged from the case study is that one can sacrifice a modest amount in the economics so as to improve the environmental impact. This was done by replacing steam reforming by biomass gasification and not using compressed gas for storage. We include the manuscript that has emerged from this work.

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 addressed the problem where a network of candidate processes is given over a specified time horizon described by multiple time periods in which product demands are specified. The 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 mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints. For simplicity he assumed that the time required for a pilot plant study corresponds to one time period. To solve this problem Bora developed a dual Lagrangean branch and bound method. He 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. 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 10 tons/day and making an additional expansion of 4.49 tons/day at period 1 if the yield turns out to be 69%. If the yield for Process I is 81% then an expansion of 2.98 tons/day is made also in period 1.

For the deep-water oilfield development problem, Bora has considered a number of reservoirs where each contains several possible well sites. Some of these 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 can be either a small FPSO, converted from a retiring oil tanker, or a large FPSO, newly constructed grassroots facilities. An FPSO can produce, store and offload the produced oil to other tankers. Unlike FPSO, a TLP cannot produce oil; it possesses only drilling and oil recovering capability. TLP and FPSO facilities can be connected 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. 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. The uncertainties are in the sand quality, size of the reservoir and breakthrough time. The goal is to maximize the expected net present value of the project.

Bora has developed in cooperation with Vikas Goel from ExxonMobil an MINLP model with a 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. In the proposed model the 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. 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 essentially the same, except that each subproblem is solved using BARON as the global optimization algorithm. Since this greatly increases the computational expense Bora has developed a hybrid scheme where only the first and last subproblems are solved to global optimality, while the intermediate iterations are solved with the outer-approximation algorithm (OAA in AIMMS).

Bora has also implemented the method using a special scheme for subgradient optimization to update the Lagrange multipliers. He considered first the case of one reservoir with linear production profile over a 10 year period. The best solution from the stochastic program had an expected NPV of $\$6.37 \times 10^9$ which is higher than the expected value (mean value) solution ($\$5.81 \times 10^9$). In the optimal solution, the model predicts start building two small FPSO facilities, one TLP and drilling 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). Bora also solved a problem with a nonlinear profile in which the maximum net present value of the stochastic program obtained was $\$4.59 \times 10^9$ versus $\$3.76 \times 10^9$ of the expected value. As for computational requirements the first problem required 3.6 hrs of CPU-time with the hybrid scheme vs. 9 hrs when global optimization is applied at each iteration. In the second problem the computing time was reduced from 120 hrs down to only 2.6 hrs. The manuscript describing this work is listed at the end of the newsletter. Bora is producing another one on the hybrid strategy.

In addition to the above work, Bora has continued 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. Bora has developed 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 to 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 is in the process of writing a manuscript on this work.

Mutisite Planning and Scheduling of Multiproduct Plants

New developments: **Spatial and temporal Lagrangean decomposition**

Students: **Sebastian Terrazas Moreno [Ph.D. started on Jan 2008]**
Philipp Trotter [RWTH-Aachen student, started on Jan 2009]

The initial problem that Sebastian 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 Erdirik 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 this project is to see if one can theoretically prove that temporal decomposition is always superior, which is a conjecture that we believe is true. Philipp Trotter, an exchange student from RWTH-Aachen will work on this project under the supervision of Sebastian.

Integrated Chemical Sites subject to Discrete and Continuous Uncertainties

New developments: **MILP formulation for maximizing expected stochastic flexibility**

Students: **Sebastian Terrazas Moreno [Ph.D. started on Jan 2008]**

This is a new Enterprise-wide Optimization project in collaboration with John Wassick from Dow Chemical. The project was defined during a one-month internship by Sebastian in Freeport. The problem consists of an integrated site that is composed of a highly interconnected network of processes that manufactures final products and intermediates. Uncertainties are considered in the demand of products and in the availability of raw materials in the form of continuous distribution functions. Discrete uncertainties are also considered for the failures of processes that lead to temporary shut-downs. Each failure is characterized by mean time between failures (MTBF), mean time to repair (MTTR), and standard deviation of time to repair (SDTTR). The problem consists in determining: (i) number and capacity of redundant processes, (ii) total capacity, and set point for intermediate storage tanks, and (iii) capacity expansion of existing processes. The objectives are on the one hand to maximize net present value (or minimize cost), and on the other hand to maximize the probability of feasible operation. In order to address this bi-criterion optimization problem Sebastian reformulated the problem as a parametric program where the *expected stochastic flexibility* is maximized subject to subject to capital investment available at some level. We should note that the concept of *expected stochastic flexibility* was developed by David Straub as a framework for integrating discrete and continuous uncertainties. The basic idea consists of considering discrete states s, each with a given probability, and each with an associated stochastic flexibility, which corresponds to the probability of feasible operation, which in turn requires the solution of a multiple integral over a set of inequalities.

Sebastian has developed a superstructure in which the possibility of adding intermediate storage tanks is included, as well as the capacity expansion of processes. Also, instead of considering variable points inside the feasible region for the integration of the continuous distribution functions, Sebastian considered a fixed number of points placed in the domain according to a Gaussian quadrature formula. This has the advantage of keeping the model linear since the maximization of the expected stochastic flexibility can then be formulated as an MILP problem. Also, the mean residence time in a state s is was approximated as the time to repair. Sebastian has explored this idea with a small process network by Straub consisting of 4 processes and 3 chemicals. If no investment is available the model predicts an expected stochastic flexibility of 0.815. By increasing the capital available the Pareto curve converges asymptotically to 0.96. In all cases no capacity expansion was performed, but only addition of storage capacity.

Design and Planning of Responsive Supply Chains

New Development: **Analysis of stochastic inventory management in terms of responsiveness**

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 response times that are a function of safety stocks are not taken into account. It is our major goal to establish the trade-offs between economics and deterministic and probabilistic response times or lead times.

As a first step, Fengqi addressed the long term design problem of a supply chain, for which he developed a superstructure model with dedicated and multiproduct continuous plants. The time horizons considered are of the order of years, and no inventories are considered (worst case for response). The problem was 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. 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. 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. 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. Fengqi obtained analytical expressions for triangular and normal distributions of the demands. The bi-criterion optimization model was solved with the ε-constraint method, but Fengqi developed a hierarchical algorithm for the solution of the resulting large-scale MINLP by 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's manuscript reprint is included in this newsletter.

Fengqi has also analyzed the project on multiechelon stochastic inventory management from the point of view of responsiveness, and concluded that the guaranteed service approach represents an upper bound to the expected lead time.

Supply Chain Optimization under Uncertainty

New Development: **MILP model for capacity planning with reactor transformation and construction lead time**

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

As indicated in the last newsletter, this was a collaboration project with Dow Chemical in the context of the Enterprise-wide Optimization. The major goal was 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. 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 accepted for publication and is listed at the end of the newsletter.

As a second step, Fengqi has been considering 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. Fengqi has 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: Large-scale supply chain design with multi-echelon stochastic inventory

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

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. The reprint on this work is included in this newsletter.

Fengqi 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 150 customers are presented to illustrate the performance of the algorithm. Fengqi' manuscript is listed at the end of this newsletter.

Stochastic Vehicle Routing and Tank-sizing

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

Students: Fengqi You [Ph.D. started Jan 2006]
Elisabet Capon [UPC, Barcelona, Sept-Nov 2008]

This is a 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 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. To improve the computational efficiency of the detailed routing problem, Elisabet and Fengqi have developed a simultaneous route selection and tank sizing model. The model still captures the tradeoff between capital cost of tank sizing and the operating cost of vehicle routing, while simultaneously predicts the optimal tank size for each customer and the routes to be used in the detailed routing. Using only the routes selected by this model, the detailed routing problem can be solved effectively without the need to explore all the alternative routes between customers. Computational study of a toy problem shows that this method can save more than 20% CPU time for solving the detailed routing problem. After deciding the most effective deterministic model, the next step of this project will be to address uncertainties in demands, and the loss or addition of customers over time.

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 is working on a Enterprise-wide Optimization 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 given potential number of priority-base slots. The proposed approach consists of assigning specific transfer operations to the ordered set of slots. The objective used is to maximize the gross margins of crudes that need to be processed to satisfy given demands. By introducing 0-1 variables for assignments, and continuous time, volume and level variables, and imposing 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. This is of course is only true for the objective of maximizing the gross margins of distilled mixed oil.

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 applied this solution approach to several problems from the Lee et al. (1996) paper obtaining very encouraging results. In the smallest problem the proposed method is one order of magnitude faster than DICOPT and two orders of magnitude faster than BARON. As for the solution of the four problems, in three of them the gap was 0%; the one that was not had a gap of 3.3%. The computing times ranged between 2 sec and 82 sec. The manuscript describing this work is listed in this newsletter.

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). Sylvain used this approach on the Lee et al. (1996) problems where the objective is to minimize logistics costs, including 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.

Finally, Sylvain, is also developing generalizations of scheduling models beyond the crude oil problem, based on representations that range from single-operation and multiple-operation sequencing.

Planning of Refinery Operations

New development: **Modeling and testing of 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.

Abdul initially implemented an extension of the aggregate distillation models proposed by Jose Caballero. This required the CDU to be represented through cascaded columns, including columns with steam stripping. The initial aggregated model, however, did not include steam stripping. It was tested in a mixture with 10 to 20 hydrocarbons in conventional distillation columns. Since this led to significant convergence problems, often yielding infeasible NLP solutions, 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 improved the robustness of the solution of the NLPs. Abdul was 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 columns. Initial attempts to use several common models were not successful in overcoming convergence problems. Moreover, we also found surprisingly little in the literature on how to model these columns as they can be regarded as absorbers. After many trials Abdul has developed 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 for the equilibrium calculations. Optimizations of tindividual steam strippers have proved to be fairly robust and accurate. Abdul is now implementing this model as part of the cascaded columns in order to represent the CDU column. The next phase will involve the use of pseudo-properties for handling real crudes.

Planning for Petroleum Allocation

New development: Multidimensional knapsack constraints

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

This project involves Roger Rocha from Petrobras, who is visiting the CAPD for two years, regarding applications in Enterprise-wide Optimization. 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 that 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. The manuscript describing this work is listed in this newsletter.

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. Roger has recently extended this work with "cascading" multidimensional knapsack constraints that can be obtained by reformulation of certain mass balances in supply chain problems. The importance of these constraints is that Roger has been able to develop facets for some particular cases, and valid inequalities for the general case. He is now in the process of testing these structures and cuts.

In another 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. The computational results on the petroleum allocation problem have not proved to be as encouraging, although one still obtains reductions of the order of 20-30%.

Cost Model for a Multiproduct Process with Multiple Stages

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

Ricardo started a new project on Enterprise-wide Optimization with the PPG Glass Business and Discovery Center (GBDC) with the aim of developing a mathematical model for the planning and scheduling of the production of spectrally selective tinted glasses. The process is defined as a multiproduct continuous process with considerable large sequence dependent changeover times and with a subset of products without changeover times. This project involves three stages of development: 1) development of a simplified model that captures the main essences of the process; 2) improvement of the previous model by considering the impact of the management of subproducts in the scheduling; 3) development of a detailed model where the products are defined by all the characteristics of each SKU. Ricardo has been developing a mathematical model for the first stage, and studying different approaches to efficiently handle the size and complexity of the Mixed Integer Linear Programming (MILP) model that described the planning and scheduling of the production line for extended time horizons. The main focus has been on the improvement of existing models (Erdirik-Dogan and Grossmann, 2006) and on the study of generic and efficient solution strategies. At the model level, two MILP submodels to consider transition times and minimum run lengths across time periods have been developed. At the moment two solution approaches have been studied a bi-level decomposition and a forward rolling horizon approach. In addition, a rigorous aggregation of the products at the scheduling level was developed in order to decrease the combinatorial complexity of the model.

Scheduling of Batch Multiproduct Plants

New Development: **Scheduling of cement plants with variable electricity cost application of Dinkelbach's algorithm in cyclic scheduling**

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

Pedro Castro spent four months at Carnegie Mellon, mostly working on an Enterprise-wide Optimization project with ABB dealing with the scheduling of cement plants with variable electricity cost. In addition to this work, Pedro has been collaborating with us for a number of years developing effective computational strategies for effectively solving MILP models for large scale scheduling problems.

As indicated in the last newsletter, with input from Muge, Pedro developed 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 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.

Regarding the ABB project, Pedro considered cement plants that operate semi-continuously. In the final phase of cement manufacturing, clinker is crushed and ground together with additives to obtain cement. The grades of cement are characterized by their chemical composition and grain size distribution. The grinding process takes place in mills, which are large rotary machines with steel balls that crush the material until the right grain size distribution is reached. According to the grade, the cement is conveyed to silos, where it is stored until dispatch takes place. The energy contract signed by the plant and electricity

provider establishes a certain pricing policy. Electricity cost is typically lower during the night and higher during the day. It is also lower during the weekends. The objective in the scheduling problem is to develop a short term schedule (one week) that minimize the total energy cost subject to constraints on resource availability that includes processing units (mills), storage units (silos), and utilities (electricity). Pedro assumed full connectivity between mills and silos even though, in reality, some combinations may not be possible to occur simultaneously. It is also assumed that every silo can store all product grades, in order to increase the flexibility of the model, but only one grade at a time. Normally, the product grade allocated to a silo never changes in its entire life. Pedro developed both discrete and continuous time RTN models for this problem. The development of the continuous model was particularly challenging, although it could be simplified since changeovers were not accounted for. The results showed that the continuous time model can only solve problems of small size. The discrete-time model proved to be more effective since it had a very tight LP relaxation, which allowed it to handle a sufficiently fine time grid to represent the problem data accurately. The goal was to ensure a weekly schedule that accounted for hourly changes in electricity cost, and this has been successfully accomplished. Pedro was able to solve with the discrete model problems of industrial significance (5 mills, 3 products, 3 silos, and hourly changes of electricity cost) with optimality gaps below 1% in less than 5 minutes. Another interesting result was to show that potential cost savings of around 20% can be achieved when applying this scheduling model for cases when plant is operating at around 50% capacity. The manuscript describing this work is listed at the end of this newsletter.

Pedro has also collaborated with Fengqi in the optimization of linear fractional MINLPs, which arise in cyclic scheduling. Fengqi proved convergence properties of Dinkelbach's algorithm for mixed-integer fractional programs. This algorithm conceptually corresponds to Newton's method, although it can also be viewed as a special type of direct substitution method. Fengqi solved problems with up to 2000 0-1 variables and 2000 continuous variables and constraints requiring only about 5 minutes of CPU time. Other solvers like DICOPT, SBB and BARON cannot solve these problems. On the cyclic scheduling problem of Pedro Castro Dinkelbach's algorithm also greatly outperformed DICOPT, SBB, α-ECP and BARON. A manuscript is in preparation on this work.

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. See:
http://newton.cheme.cmu.edu/interfaces/indexwater.html

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.

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, started August 2004)**

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 investigated this past semester relies on branch-and-bound. While standard approaches relax each nonconvex term separately, Xiaowei explored relaxations of entire quadratic constraints. She developed new ways to generate cutting planes for these constraints from the convex envelopes of multilinear functions. Once these cutting planes are added to the root-node relaxation, the performance of BARON on this class of problems improves by several orders of magnitude. A related paper was submitted to *Optimization Methods and Software* and has been accepted subject to minor revisions.

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. A current focus has been on replacing BARON's previous LP relaxations by MIP relaxations, where integrality constraints are enforced on integer variables of the original, possibly nonconvex, MINLP. In a preliminary implementation, the Xpress MIP solver has been used to solve these relaxations and has more than doubled BARON's ability to solve MINLPs from the IBMLib collection of problems. The implementation is expected to be fully functional by the end of this coming semester, including a link to the Cplex MIP solver.

Global Optimization for Problems in Quantum Chemistry

Student: Mr. Keith Zorn (Ph.D. student at CMU, started September 2007)

Keith Zorn has been working on 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. This semester, Keith continued his work on additional RLT relaxations for this problem. He has found that a rather unusual relaxation (high order RLT) considerably tightens the relaxation gap and results in an approach that is over a magnitude faster than other approaches to this problem.

Global Optimization for Machine Learning Problems

Student: Mr. Xuan Shi (visiting researcher at CMU)

Xuan Shi, who first joined the group as a Master's student 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 involves 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 has been written in GAMS and a generic interface has been 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 has been compared against backpropagation, and other popular algorithms from the machine learning literature. The main conclusion thus far has been that our approach results in lower training errors and much simpler neural networks than all other approaches.

Algorithms and Software for Black-box Optimization

Student: Mr. Luis Miguel Rios (Ph.D. student in Industrial Engineering at the University of Illinois, started August 2002)

This project began with 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 20 different black-box solvers. 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. Test problems of black-box models from industry are currently sought.

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 made available in the near future.

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

Students:

Mr. Deepak Channamariyappa (former M.S. student at CMU, currently visiting researcher)
Mr. Joseph Elble (Ph.D. student in Industrial Engineering at the University of Illinois)
Mr. Yiqi Zhu (former 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 been studying of preprocessing techniques for Linear Programming. These techniques currently represent more of an art rather than science in the field of Linear Programming. The long term goal of this 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. This past semester Deepak performed computational experimentations that rely on the presolve routines of the GALLAHAD package. Our main finding was that the sequence in which different preseolve techniques are applied to any given LP problem can affect the final outcome of preprocessing, in terms of number of variables/constraints and sparsity of the presolved problem. Current work focuses on identifying an "optimal" presolve sequence.

Yiqi Zhu has been studying 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. Yiqi has implemented a simple successive linear programming algorithm under the GAMS environment. He has successfully solved a collection of over 100 small and medium test problems and compared his implementation against CONOPT. CONOPT is up to 4 times faster for QPs and 10 to 20 times faster for general NLPs. This is encouraging, given the preliminary nature of Yiqi's implementation, especially the fact that there is no preprocessing in his code and no clever restarts of LPs. The most interesting result is that nearly all problems tried are solvable by this preliminary implementation, whereas it is reported that previous SLP solvers did not fair well on a large number of problems on which they were tried.

Panagiotis Vouzis and **Joe Elble** have performed an extensive 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 and Joe implemented several iterative methods for solving LPs on the GPU. The main conclusion was that a combination of GPU/CPU implementation significantly outperforms parallel computations on a 16-node Linux cluster. A related paper has been submitted to *Parallel Programming*.

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, started September 2007)

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, has been working on 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

Students: **Saurabh Awasthi (former M.S. student at CMU)**
Danan Wicaksono (M.S. student at 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 completed his MS thesis in August 2008, 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. Danan Wicaksono is continuing Saurabh's work, with the intent to look into flexible docking, i.e., allow for flexible protein and ligand structures.

Design of Drilling Fluids for Extreme Drilling Conditions

Student: Apurva Samurda (Ph.D. student at CMU, started September 2007)

The current drilling fluids market exceeds $3 billion a year but there are no cost efficient and environmentally benign means for drilling under extreme conditions. By extreme conditions, we refer to drilling depths beyond 20,000 ft, pressures as high as 2000 bar, and temperatures as high as 250 °C. The environmental constraints include the requirement for biodegradable fluids that are not toxic to aquatic environments. There are three main families of drilling fluids currently in use: gaseous, aqueous, and non aqueous. The major driver of the drilling fluids market is that different well conditions require different types of drilling fluids to be used for most effective operation. The drilling fluid should possess a number of properties: (1) it should gel under static conditions so as to keep the cuttings suspended when the fluid is not moving; (2) it should have high shear thinning and sufficiently high viscosity for efficient hole cleaning; (3) it should have high annular velocity, which improves transport of cuttings; (4) it should have density that provides a hydrostatic pressure just sufficient to prevent collapse of weak formations into the borehole; (5) it should have suitable pH in order to reduce corrosion; and (6) it should be environmentally benign, i.e., it should have good biodegradability and low aquatic toxicity. It is important to recognize that an optimal drilling fluid must be determined as a function of well *and* drilling conditions. A major challenge for the design of drilling fluids for extreme drilling is that the fluid must be stable under a very wide range of operating conditions. Furthermore, the fluid must be optimal from an economic standpoint, while having minimal environmental impact. Another major challenge is that the behavior of fluids under extreme conditions is very difficult to predict computationally. Indeed, existing fluid mixture models are complex and highly nonlinear. Since viscosity is one of the primary concerns in the context of drilling fluids, attention of this project has focused on viscosity prediction models. In addition, Apurva has proposed molecular design via an optimization formulation that relies on the inversion of nonlinear property relationships so as to avoid nonlinearities in the underlying property prediction models. In recognition of the fact that drilling fluids are blends, Apurva will be extending these optimization models from the design of pure fluids to blends. Data will be collected from industrial use of drilling fluids in order to calibrate these models. A mathematical model will be developed that will integrate molecule and mixture design with the post-drilling process, i.e., filtering and recycling of the fluid in order to identify and design fluids that minimize environmental impact as well as drilling costs. Finally, optimization algorithms will be developed for handling the nonlinearities that arise in this model from mixture design considerations.

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

Adaptive Control Systems

New developments: Software for adaptive PID control. Software for transfer function identitifaction

Students: Richard Chan (Post Doc researcher and ILS)
Keyu Li (PostDoc researcher and ILS)

Keyu Li has developed a software solution for passivity based adaptive feedforward control and automatic tuning of PID controllers. The algorithm is based on a fast algorithm for global optimization to identify first

order deadtime models suing real time data and the method to select informative data developed by Wayo in his PhD thesis. The feedforward gains are tuned continuously whereas the feedback (PID) controller gains are updated only intermittently. The PID algorithm is based on fixing the gain and phase margins (user specified) and them optimizing the bandwidth. These problems are solved on-line and provide a novel and robust solution to the adaptive PID control problem. 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 and is ready for testing in industrial trials. Richard Chan has been working on developing a multivariable adaptive predictive controller which is configurable on the fly. The algorithm uses a classical MPC formulation to define the control signal whereas the models are based on a Laguerre type model formulation which is suitable for robust adaptive control of uncertain and slowly time-varying systems. The algorithm has been tested in simple simulation studies and on the Shell challenge problem.

Modeling and Nonlinear Control

New developments: **New stability results for the reactive, multi-component distillation Continuous time switching lemma, models for chemical looping combustion. Papers submitted on adaptive control systems and nonlinear control**

Students: **Mohit Aggarwal (Ph.D. expected 2009)**
Balaji Sukumar (PostDoc)
Juan Du (New PhD Student)

Mohit has developed stability theory for systems with time-varying reference using an idea called contraction analysis. The theory has application distributed, web-based simulation and control. Mohit has used the theory to develop modeling tools for chemical process systems using invariant groups as a way to develop reduced order models for very complex reacting systems. With the help of Bala he has developed reduced order process models using process invariants for the gasifier in the IGCC process, a bio-gasifier (work with AirProducts) and the carbothermic aluminum process. Bala has used the method to develop reduced order models for a chemical looping reactor being developed by Alstohm. Juan Du has extended the infinite switching lemma developed by Wayo for continuous time systems. The lemma is useful for stability analysis of chaotic systems since it can be used to show convergence to invariant (omega-limit) sets without extensive linearization or re-normalization.

Carbothermic Aluminum Production

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

Students: **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 (PhD expected 2010)
Chengtao Wen (PostDoc Researcher)
Simon Markovski (MS expected 2009)

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.

PUBLICATIONS:

B-09-01
Lang, Y-D, A. Malacina, L. T. Biegler, S. Munteanu, J. I. Madsen and S. E. Zitney, "Reduced Order Model Based on Principal Component Analysis for Process Simulation and Optimization," submitted for publication (2008) http://numero.cheme.cmu.edu/Papers/

B-09-02
Baumrucker, B. T. and L.T. Biegler, "MPEC Strategies for Optimization of Hybrid Dynamic Systems," submitted for publication (2008) http://numero.cheme.cmu.edu/Papers/

B-09-03
V. M. Zavala and L. T. Biegler, "Nonlinear Programming Sensitivity for Nonlinear State Estimation and Model Predictive Control," submitted for publication (2008) http://numero.cheme.cmu.edu/Papers/

G-09-01
Castro, P.M., I. Harjunkoski and I.E. Grossmann, "New Continuous-Time Scheduling Formulation for Continuous Plants under Variable Electricity Cost," submitted for publication (2008). http://egon.cheme.cmu.edu/Papers/CastroIndEngChemRes2008.pdf

G-09-02
Guillen-Gosalbez, G., F.D. Mele and I.E. Grossmann, "A Bi-criterion Optimization Approach for the Design and Planning of Hydrogen Supply Chains for Vehicle Use," to appear in *AIChE J.* (2008). http://egon.cheme.cmu.edu/Papers/Guillen-Gosalbez-et-al.pdf

G-09-03
Mouret, S., I.E. Grossmann and P. Pestiaux, "A Novel Priority-Slot Based Continuous-Time Formulation for Crude-Oil Scheduling Problems," submitted for publication (2008) http://egon.cheme.cmu.edu/Papers/Mouret-IECRmanuscript-08-10-06.pdf

G-09-04
Rocha, R., I.E. Grossmann and Marcus V. S. Poggi de Aragão, "Petroleum Allocation at Petrobras: Mathematical Model and a Solution Algorithm," submitted for publication (2008) http://egon.cheme.cmu.edu/Papers/paper_FOCAPO_extended_submittedVersion.pdf

G-09-05
Sawaya, N. and I.E. Grossmann, "Reformulations, Relaxations and Cutting Planes for Linear Generalized Disjunctive Programming," submitted for publication (2008) http://egon.cheme.cmu.edu/Papers/ReformulationRelaxation-SawayaGrossmann.pdf

G-09-06
Tarhan, B., V. Goel and I.E. Grossmann, "A Multistage Stochastic Programming Approach for the Planning of Offshore Oil or Gas Field Infrastructure under Decision Dependent Uncertainty," to appear in *Ind.Eng.Chem. Res*. (2008) http://egon.cheme.cmu.edu/Papers/Tarhan_Grossmann_Goel.pdf

G-09-07
You, F. and I.E. Grossmann, "Integrated Multi-Echelon Supply Chain Design with Inventories under Uncertainty: MINLP Models and Computational Strategies," submitted for publication (2008) http://egon.cheme.cmu.edu/Papers/MLSS_SCD_paper1.pdf

G-09-08
You, F., J.M. Wassick and I.E. Grossmann, "Risk Management for a Global Supply Chain Planning under Uncertainty: Models and Algorithms," to appear in *AIChE J*. (2008) http://egon.cheme.cmu.edu/Papers/RiskMgmtDow.pdf

S-09-01
Bao, Xiaowei, N.V. Sahinidis and Mohit Tawarmalani, "Multiterm Polyhedral Relaxations for Nonconvex, Quadratically-constrained Quadratic Programs," submitted to *Optimization Methods and Software*, (2008).

S-09-02
Elble, J. and N. V. Sahinidis, Matrix Binormalization on a GPU, Lecture Notes in Computer Science, submitted.

S-09-03
Elble, J., N.V. Sahinidis, and Panagiotis Vouzis, "GPU Computing with Kaczmarz's and other Iterative Algorithms for Linear Systems," submitted to *Parallel Computing*, (2008).

REPRINTS

Ahmed, S. and N. V. Sahinidis, "Selection, Acquisition, and Allocation of Manufacturing Technology in a Multi-product Environment," *European Journal of Operational Research*, 189, 807–821, (2008).

Baumrucker, B.T., J. G. Renfro and L.T. Biegler "MPEC Problem Formulations in Chemical Engineering Applications," *Computers and Chemical Engineering*, 32, pp. 2903-2913 (2008).

Caballero, J.A. and I.E. Grossmann, "An Algorithm for the use of Surrogate Models in Modular Flowsheet Optimization," *AIChE J.* 54, 2633 - 2650 (2008).

de Prada, C., I. E. Grossmann, D. Sarabia and S. Cristea, "A Strategy for Predictive Control of a Mixed Continuous Batch Process," *Journal of Process Control* 19, 123–137 (2009).

Erdirik-Dogan, M. and I.E. Grossmann, "Simultaneous Planning and Scheduling of Single-Stage Multiproduct Continuous Plants with Parallel Lines," *Computers and Chemical Engineering* **32**, 2664-2683 (2008).

Flores Tlacuahuac, A. and L. T. Biegler, "Integrated Control and Process Design during Optimal Polymer Grade Transition Operations," *Computers and Chemical Engineering*, 32(11), pp. 2823-2837 (2008).

Flores Tlacuahuac, A., S. Terrazas Moreno, and L. T. Biegler, "On Global Optimization of Highly Nonlinear Dynamic Systems," *I & EC Research*, 47, 8, pp 2643 - 2655 (2008).

Guillen-Gosalbez, G. and I.E. Grossmann, "Optimal Design and Planning of Sustainable Chemical Supply Chains under Uncertainty," *AIChE J*., 55, 99-121 (2009).

Karuppiah, R. and I.E. Grossmann, "A Lagrangean Based Branch-and-Cut Algorithm for Global Optimization of Nonconvex Mixed-Integer Nonlinear Programs with Decomposable Structures," *Journal of Global Optimization* 41, 163 (2008).

Karuppiah, R. K.C. Furman and I.E. Grossmann, "Global Optimization for Scheduling Refinery Crude Oil Operations," *Computers & Chemical Engineering* 32, 2745–2766 (2008).

Parag Jain, M. S. Jhon and L. T. Biegler, "Optimization of Polymer Electrolyte Fuel Cell Cathodes," *Electrochemical and Solid-State Letters*, 11(10), pp. B193-B196 (2008).

Perez-Correa, J. R., C. Gelmi, L. T. Biegler, "Dynamic Optimization," in Optimization in Food Engineering, F. Erdogdu (ed.), pp. 229-253, CRC Press (2008).

You, F. and I.E. Grossmann, "Design of Responsive Process Supply Chains under Demand Uncertainty," *Computers & Chemical Engineering*, 32, 3090-3111 (2008).

You, F. and I.E. Grossmann, "Mixed-Integer Nonlinear Programming Models and Algorithms for Large-Scale Supply Chain Design with Stochastic Inventory Management," *I&EC Research* **47**, 7802–7817 (2008).

Zavala, V., M., C. D. Laird and L. T. Biegler, "A Fast Computational Framework for Large-Scale Moving Horizon Estimation," *Journal of Process Control*, 18(9), pp. 876-884 (2008).

Zavala, V. M.; and Biegler, L.T. "Large-Scale Nonlinear Programming Strategies for the Operation of Low-Density Polyethylene Tubular Reactors," in *Computer Aided Chemical Engineering*, 25, pp. 629-634, B. Braunschweig and X. Joulia (eds.), *Elsevier*, Amsterdam (2008).

Zavala, V. M., C. D. Laird and L. T. Biegler, "Interior-Point Decomposition Approaches for Parallel Solution of Large-Scale Nonlinear Parameter Estimation Problems," *Chemical Engineering Science*, 63, pp. 4834-4845 (2008).