



***CENTER FOR ADVANCED PROCESS
DECISION-MAKING***

New Directions for Process Systems Engineering

**Lorenz T. Biegler
Ignacio E. Grossmann
Steinar Hauan
Gary Powers
B. Erik Ydstie**

*Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213*

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TABLE OF CONTENTS

General News	2
Executive Summary	4
Status of Research Projects	
<u>Larry Biegler's Group</u>	
<i>General Frameworks for Large Scale Optimization Strategies and Applications</i>	7
<i>Mathematical Programs with Equilibrium Constraints (MPECS)</i>	8
<i>Simultaneous Optimization of Differential-Algebraic (DAE) Systems</i>	9
<i>Large-Scale Optimization for Fuel Cell Models</i>	10
<i>Reduced Order Models for PDE-based Units in Power Plant Flowsheets</i>	11
<i>Optimization and Control of Periodic Adsorption Processes</i>	11
<u>Ignacio Grossmann's Group</u>	
<i>Open Source Code for MINLP Optimization</i>	12
<i>Algorithms for Nonlinear Disjunctive Programming</i>	13
<i>Global Optimization of Integrated Process Water Systems</i>	15
<i>Optimal Design of Corn-based Ethanol Plants</i>	17
<i>MINLP Flowsheet Optimization with Process Simulators</i>	18
<i>Synthesis of Crystallization Processes</i>	18
<i>Design for Sustainability</i>	19
<i>Design and Planning of Deep-Water Oilfield Development under Uncertainty</i>	19
<i>Simultaneous Planning and Scheduling of Continuous Multiproduct Plants</i>	21
<i>Design and Planning of Responsive Supply Chains</i>	22
<i>Scheduling of Batch Multiproduct Plants</i>	23
<i>Simultaneous Scheduling and Control</i>	24
<i>Software for MINLP Optimization in Design and Scheduling</i>	24
<u>Steinar Hauan's Group</u>	
<i>Agent Systems in Engineering Design and Optimization</i>	25
<i>Microscale Chemical Synthesis and Sensing</i>	26
<i>Microscale Total Analysis Systems</i>	27
<i>A MEMS-based Gravimetric Biosensor</i>	27
<i>Design of Multiproduct Reactive Separation Plants</i>	28
<u>Erik Ydstie's Group</u>	
<i>Modeling and Control of Distributed Process Networks</i>	29
<i>Modeling and Control of Particulate Processes</i>	30
<i>Supervised Adaptive Control</i>	30
<i>Passivity Based Control of Multi-Phase Reactor Systems</i>	31
<i>Thermodynamics and Process Networks</i>	31
Publications	32
Reprints	33

GENERAL NEWS

We would like to welcome our new member to the CAPD, the Collaboratory for Process & Dynamic Systems Research (NETL). The contacts will be Prof. Richard Bajura from the National Research Center for Coal and Energy (NRCCE) of West Virginia University and Dr. Steve Zitney from the Office of Research & Development in NETL.

Ignacio Grossmann was elected Director of AIChE, and will serve for a three year term. He visited Tsinghua University in Beijing, China, from September 2-10, 2006, where he gave one seminar and two lectures. He also gave a seminar in the Department of Industrial and Systems Engineering, University of Wisconsin, Madison, and the keynote address, "Research Challenges in Process Systems Engineering: Product and Process Design, Energy and Sustainability, Enterprise-wide Optimization," at the 3rd Interamerican Congress of Chemical Engineering that took place in Buenos Aires on October 2-4, 2006. He also participated in the NSF workshop on Cyberinfrastructure for Chemical and Biological processes that took place from September 25-26. Ignacio was also recently appointed to the Advisory Board of the Office of International Engineering and Science at NSF.

Larry Biegler just returned from a short sabbatical, where he was a Fulbright fellow at the University of Heidelberg. In addition to invited seminars at the universities in Heidelberg, Magdeburg, Dortmund and Dresden, he was the first Simon Stevin Lecturer in Engineering Optimization at Katholieke Universiteit Leuven. He was also a plenary speaker at the Fast NMPC IFAC Workshop in Grenoble, France and the Veszprém Optimization Conference: Advanced Algorithms (VOCAL) in Hungary.

Erik Ydstie gave the 2006 Annual Sargent Lecture on Process Systems Engineering at Imperial College in December. He talked about Inventory and Flow Control in Process Networks. The lecture is posted at the Imperial College web-site. Industrial Learning Systems has obtained an R&D contract with Emerson Process Management, Power and Water Solutions here in Pittsburgh to develop software and interfaces for adaptive control of superheaters in coal fired power plants. The contract allows iLS to hire two full time Ph.D. Chemical Engineers to work on product development. Keyu Li from Cleveland State University and Richard Chan from University of New South Wales in Australia are expected to join iLS in March. Erik continues his work on scale-up and design with Alcoa for the 3MW test bed system for the carbothermic aluminum project. A new contract has been obtained to fund 1 PostDoc and 1 Ph.D. student for 2007. Sudhir Narajan will join as a PostDoc in March to work on Solar Energy related project.

Congratulations to **Nick Sawaya**, student of Ignacio, who successfully defended his Ph.D. in November and joined ExxonMobil, Corporate Research. Congratulations to **Eduardo Dozal-Mejorada**, student of Erik Ydstie, who received the Geoffery D. Parfitt Memorial Award and, **Yoshiaki Kawajiri**, student of Larry, for receiving the Symposium Award at the CHEGSA Symposium that took place on October 20-21, 2006. Congratulations to **Victor Zavala, Scott Turnberg and Bora Tarhan** who passed their Ph.D. proposals. Congratulations also to **Anshul Agrawal** and **Parag Jain**, students of Larry, **Fengqi You** students of Ignacio, and **Mohit Aggarwal**, student of Erik who recently passed their Ph.D. qualifying exams.

Congratulations to **John Siirola** (Ph.D., S2005) won the Best Paper award chosen by the editorial board of Computers and Chemical Engineering for his paper entitled "Computing Pareto Fronts using distributed agents".

Congratulations to **Mike Bartkovsky** (Aug) and **Murni Ahmad** (Oct) who both successfully defended their Ph.D. thesis and are now alumni of the groups. Mike is going to Bayer (Houston, TX) while Murni has accepted a teaching position at Universiti Teknologi PETRONAS in her home country of Malaysia. Congratulations to **Scott Turnberg** who has passed his Ph.D. proposal exam.

This year the Chemical Engineering Department recruited a class of 30 graduate students, which has produced the addition of a large number of students in the PSE area. It is a pleasure to welcome the following new Ph.D. students to the PSE group: **Rui Huang** from Zhejiang University, **Lin Weijie** from Tsinghua University, and **Sree Rama Raju Vetujori** from Jawaharlal Nehru Tech. University will be working with Larry Biegler; **Ravi Kamath**, from

IIT-Bombay, and **Adam Malacina** from IIT-Chicago, will be working under the joint supervision of Larry and Ignacio; **Abdulrahman Alattas** from the Petroleum Institute in Abu Dhabi and Colorado School of Mines, **Sylvain Mouret** from Ecole Polytechnique in Paris and **Juan Ruiz** from Instituto Regional in Rosario Argentina, will be working with Ignacio Grossmann; **Michael Wartmann** from University of Stuttgart who will be working for Erik Ydstie on optimal control of networked systems. The M.S. students are **Gaurav Bansal** from Coimbarore Inst. of Tech., Anna University will be working with Larry and **Vishnu Chapalamadugu** from Dr. B.V. Raju Institute of Technology will be working with Erik.

Victor Zavala and **Brian Baumrucker** spent the summer at ExxonMobil Chemicals at Baytown, TX; Victor was working on NMPC applications with detailed process models while Brian was exploring and extending complementarity models for real-time optimization. **Ramkumar Karupiah** went to ExxonMobil Corporate Research this summer and worked in the group of Kevin Furman developing MINLP scheduling models. **Bora Tarhan** spent two months in ExxonMobil, Upstream Research, working with **Vikas Goel** and Amr-El Bakry on the design and planning of offshore platforms. **Scott Turnberg** spent the summer at Dow in Midland working with John Wassick in the area of agent-based systems. **Muge Erdirik** spent one month in Midland working with John Wassick developing planning and scheduling models for batch plants. **Christy White** went to FLUOR in Los Angeles to work on the scale up of the fluid bed reactor for making solar grade silicon. The models she has developed plays a critical role on the design of the commercial system which is going to be built for REC late 2007. **Eduardo Dozal** spent three months at Shell working in distributed and decentralized MPC.

Professors Arturo Jimenez and **Vicente Rico-Ramirez**, both from Instituto de Celaya in Mexico continue spending their sabbatical year at the department with the PSE group as Fulbright scholars. Arturo's Ph.D. student **Jose Ortega** has also joined him. **Euclides Almeida Neto** from Petrobras continues to spend a year in Larry's group working on on-line dynamic optimization. **Mariano Martin** from the University of Salamanca, Spain, visited Ignacio's group working on bioethanol from August to November, 2006. **Gonzalo Guillen**, graduate from Polytechnic University of Catalunya and recipient of a Fulbright scholarship, has joined Ignacio's group as a postdoctoral fellow, and will be working in the areas of Sustainability and Enterprise-wide Optimization.

Professor Jie Bao, who was visiting Erik Ydstie's research group on his sabbatical leave from University of New South Wales in Sidney Australia, completed a joint paper with Erik and Kendell on plant wide control using passivity based control theory. He also was able to finish two more chapters on his book on passivity based process control with Prof. Peter Lee. A joint research program with Prof Bjarne Foss at NTNU in Norway on research in the area of petroleum reservoir modeling and control in the Arctic has been initiated.

CAPD e-News. We sent on October 27 our fourth e-newsletter. As we indicated previously, we now issue on a yearly basis two extensive newsletters with detailed descriptions of the projects in August and January, while the two others are brief e-Newsletters in April and October that contain short announcements as well as information that we think will be useful to the CAPD members. We would appreciate receiving feedback or suggestions for improving the e-Newsletter.

2006 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on **March 12-13, 2007**. The first day of the meeting will consist of overviews given by Larry, Ignacio, Erik, Steinar and Gary, followed by a discussion with industrial participants, and a poster session by the students. As we did last year, we will have a reception on Sunday evening, March 11, at the Danforth Lounge, University Center, and a group dinner on Monday, March 12, at Monterey Bay Inn. The second day is devoted to final year student presentations. As a special feature this year there will be a session on modeling systems on Tuesday, March 13, 2:00-4:30PM, in which representatives from GAMS, Dash Optimization and AIMMS will be describing and demonstrating their software. This session is actually part of the Enterprise-wide Optimization project (see next section), but will be open to all CAPD members.

The detailed agenda of the meeting will be sent very soon. Also, if you are interested in giving a short presentation or you have any suggestions for the format of the meeting, please let us know.

ENTERPRISE-WIDE OPTIMIZATION INTEREST GROUP

The CAPD has established the special interest group on Enterprise-wide Optimization that is part of the project "**Computational Models and Algorithms for Enterprise-wide Optimization (EWO) of Process Industries**" that has been funded by the Pennsylvania Infrastructure Technology Alliance. The current participating companies are ABB, Air Products, BP America, Dow Chemical, ExxonMobil, and NOVA Chemicals. 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: **Jeff Linderoth**; UPitt: **Andrew Schaeffer**). The next meeting of this group will take place on **March 13-14**, immediately following the CAPD Meeting. As indicated above the EWO meeting will start at 2:00PM with the special session on modeling systems. Companies who might be interested in joining this group in fiscal year 2007, 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/>

2007 CAPD SHORT COURSE <http://capd.cheme.cmu.edu/shortcourse.html>

The course this year is scheduled on June 6-12, 2007, and will be organized in three modules:

- a) Conceptual Design - taught on Wednesday and Thursday (June 6-7), with focus on process synthesis, particularly azeotropic and reactive distillation, and design of micro-scale systems.
- b) Optimization - taught on Friday and Saturday (June 8-9), with focus on modeling and algorithms for nonlinear programming and mixed integer programming including disjunctive programming and applications to process optimization.
- c) Process Operations - taught on Monday and Tuesday (June 11-12), with focus on differential/algebraic models for real time optimization and parameter estimation, and on mixed-integer programming models for process scheduling and supply chain management.

CAPD members can take one, two or all three modules and receive a 25% discount.

The detailed contents are described in: http://capd.cheme.cmu.edu/shortcourse_details.htm

The course includes extensive workshops where participants obtain hands-on experience with various software packages. Course materials include extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." For next year the course will be offered on **June 6-12, 2008**. The course can be taken in any combination of modules. A detailed description of the modules can be found in <http://capd.cheme.cmu.edu/shortcourse.html>. If you are interested in attending this course next summer, please contact Toni McIltrout at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

VIRTUAL LIBRARY ON PROCESS SYSTEMS ENGINEERING

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

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that the CAPD newsletter is distributed in electronic form. We would appreciate receiving feedback from our member companies of 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. We plan to update and modify our website in the next few months. 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>, Steinar's <http://www.andrew.cmu.edu/user/steinhau/>. 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.

Through the recent PhD of **Shiva Kameswaran**, the simultaneous approach for dynamic optimization has been analyzed through a detailed convergence analysis and large-scale optimization tools have enabled the efficient solution of these problems. A reprint that summarizes these developments is listed below. Dynamic optimization tools, ultimately for on-line use, have been applied that are centered on IPOPT, which continues to be developed at IBM. **Victor Zavala** has made strong advances in parameter and system identification for large-scale polymerization processes. This is described in a reprint listed below. In addition, Victor and **Carl Laird** have developed a formulation for Nonlinear Model Predictive Control (NMPC) that extends the work of Bock and coworkers to the simultaneous approach. As a result, large dynamic optimization problems used for NMPC and moving horizon estimation (MHE) have *on-line computation costs reduced by two orders of magnitude!* A paper that describes this work is listed below. Related to this work is the development of specialized decomposition strategies within the IPOPT framework. Finally, for periodic adsorption applications, **Yoshi Kawajiri** is currently exploring optimization strategies for Simulated Moving Bed applications, the liquid-solid analog of PSA. In previous work, he has shown substantial improvements in productivity for these systems through an efficient dynamic optimization formulation. As a follow-on to this work, two papers are listed that describe a extended optimization formulations for this challenging problem.

Enabling Software From Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the interior point nonlinear programming algorithm, IPOPT, in a number of directions. **Andreas Wächter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, based on many of our earlier SQP concepts. In the general purpose framework, it adopts a sparse decomposition of the KKT matrix, and has been tested on thousands of applications with up to a quarter of a million variables. It has also been used to solve problems that incorporate a number of specialized decomposition strategies and for a wide variety of applications with up to 2 million variables. IPOPT is available under an Open Source software license and the source code can be downloaded from <http://www.coin-or.org/Ipopt/index>.

Carl Laird and **Andreas Wächter** have rewritten IPOPT as an object-oriented code written in C++. The resulting C++ package was released for public distribution last August and was recently updated last month to version 3.2.1. The code contains a much simpler interface to modeling environments as well as a more efficient implementation of the algorithm. Finally, the object-oriented code allows for greater flexibility, especially in adopting additional linear solvers and advanced decomposition strategies.

The IPOPT code has already been interfaced to a number of modeling systems including:

- **AIMMS** –This GAMS-like system has a number of extended features including a full graphical user interface for the development of specific user applications. Moreover, it provides exact first and second derivatives and exploits the full capabilities of IPOPT. **Yi-dong Lang** has nearly completed the interface to this system and is currently testing the interface. A similar interface to GAMS is also planned for January.

- **AMPL** – This GAMS-like system is the standard development platform in the Biegler group, has been available for the past two years and can be downloaded from the COIN-OR webpage. It has extensive features for linking to MATLAB and other environments in Unix and Windows. It also provides exact first and second derivatives and exploits the full capabilities of IPOPT.
- **CAPE-OPEN** – IPOPT has been developed under the MINLP object class and has been demonstrated with the CO-Tester. A paper that describes this interface along with a reprint is listed below.
- **MATLAB** – **Claas Michalik** and **Steinar Hauan** developed an IPOPT object that directly links to MATLAB. This object accepts exact first and second derivatives and exploits the full capabilities of IPOPT. Testing of this interface is currently underway.
- **Bonmin** – As described below, joint work with researchers at IBM, Tepper as well as Ignacio's and Larry's groups have integrated IPOPT and CBC to develop a public domain MINLP code. Developed principally by Dr. Pierre Bonami, the code has been tested on a suite of convex and nonconvex MINLP problems and is being public released.

In addition, **Yi-dong Lang** has developed a user-friendly version of dynamic optimization methods. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called *DynoPC*, runs under Windows with a GUI interface. It has been distributed to several CAPD members and parts of it can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include updated versions of IPOPT and will be enhanced further by the development of a number of interfaces to optimization modeling platforms including CAPE-OPEN.

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

In the area of optimization **Nick Sawaya** completed his Ph.D. degree with exciting breakthrough work that theoretically relates Generalized Disjunctive Programming with disjunctive programming by Balas. Major outcome is a theoretical framework for obtaining stronger relaxations than the previous convex-hull by Lee and Grossmann. In collaboration with **Larry Biegler**, **Gerard Cornjuelos** and **Pierre Bonami** the open source code *bonmin* for MINLP optimization, that implements the branch and bound, outer-approximation and LP/NLP based branch and bound method, is now available in the COIN-OR library. Current work includes with **Pietro Belotti** involves exploring extensions for handling of nonconvexities. **Aldo Vecchietti**, work on LOGMIP for disjunctive programming has been incorporated in the latest version of GAMS (<http://www.ceride.gov.ar/logmip/>).

In the area of process synthesis **Ramkumar Karupiah** has completed the paper on a novel method for the global optimization that relies on Lagrangean cuts for the synthesis of integrated process water systems that must operate under multiple scenarios for varying loads of contaminants. In a joint collaboration project with **Cargill**, **Ramkumar Karupiah** and **Mariano Martin** found through synthesis and optimization techniques a design for a dry-grind corn-based ethanol process that reduces the steam consumption by 65%, and reduces the manufacturing cost by 11%. **Jose Caballero** completed a manuscript on flowsheet optimization with implicit models and complex cost and size functions using process simulators. **Ricardo Lima** has been developing an aggregated superstructure optimization approach based on MINLP for separation processes based on crystallization. **Gonzalo Guillen** has started to explore the development of a bicriterion optimization of process flowsheets and process networks in which the two criteria being optimized are economics and the eco-indicator as a measure of sustainability.

Bora Tarhan, has developed an MINLP multistage stochastic programming model and preliminary solution procedure for the design and planning of oil infrastructure planning under uncertainties in the sand quality, size of the reservoir and breakthrough time, which are represented by discrete distributions. **Muge Erdirik** is completing the work in collaboration with Dow as part of the EWO project a new continuous time model for the scheduling of parallel reactors. She has developed a novel aggregated planning model that provides very tight bounds for sequence-dependent changeover times. **Fengqi You**, has developed in a new project in Enterprise-wide Optimization MILP and MINLP models for optimizing responsiveness in supply chains for dedicated and multiproduct plants. **Pedro Castro** has completed the manuscript on formulations for single and multistage problems with parallel units for handling changeovers. In a collaboration with **Antonio Flores-Tlacuahuac** from Mexico, he has developed a new simultaneous optimization model for the combined scheduling and dynamic optimization of multiproduct CSTR reactors with sequence dependent transitions. Finally, **Rosanna Franco** has

been developing a new interface that implements the global optimization of integrated water systems by Ramkumar Karuppiah.

Steinar Hauan's Group

It has been a quiet fall semester in the Hauan group with most of the efforts going toward analysis and implementation.

The most groundbreaking result has been obtained by **Scott Turnberg** who appears to have cracked a long standing problem of automatic initialization and subsequent optimization of reactive separation cascades. Even for feasible problem specifications, it is not obvious how to initialize the internal composition profiles in such a way that the optimizer won't get stuck in infeasible solutions. Scott has used the unstable branch of reactive pinch point curves to automatically generate a set of linear constraints that limits the amount of reaction turnover on each stage as a function of composition and cumulative conversion in a cascade section. This appears to enable the automatic initialization of hundreds of columns and thus opens for the study of pareto fronts trading the cost of capital, energy and reactive holdup volumes in a systematic fashion.

Erik Ydstie's Group

Kendell Jillson has developed very efficient methods for how to model and integrate very complex process networks in a stable manner. He has developed methods that show how such systems can be designed to be self-stabilizing and self optimizing. He has also investigated the stability and control of supply chain network systems, and is also now beginning work on a project in collaboration with WVU and DOE-NETL on the modeling and control of an integrated gasification combined-cycle (IGCC) power plant. Also, Kendell will soon begin writing his Ph.D. thesis, anticipating completion and defense in late March/early April.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: Carl Laird (Ph.D. completed August, 2006)

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 addition, 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. Such networks are typically over several hundred to many thousands of nodes and require the incorporation of both spatial and temporal behavior. This difficult problem was reformulated as a DAE system with time delays. Moreover, because the hydraulic equations could be decoupled from the species mass balance, a novel preprocessing strategy renders the nodal constraints to be *linear* and the resulting problem can be solved easily using our simultaneous optimization strategies for dynamic optimization (see below). By exploiting the structure of these networks, discretized problems that represent actual municipal networks with up to 300,000 variables could be solved in only a few CPU seconds. More recently, this approach has been extended, by using an MIQP strategy, to a more robust one that promotes unique solutions. Using an efficient pre-processing step, small subproblems can be derived and attack scenarios can be identified more precisely and efficiently. This approach is described in the preprint below. Finally, the new version of IPOPT continues to be 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 multiperiod problems. These 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. Detailed results of this implementation are given in a small paper on moving horizon estimation listed below.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: **Juan Arrieta (Ph.D. started Fall, 2002)**
 Brian Baumrucker (Ph.D. started Fall, 2004)

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

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

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

Current work by **Juan Arrieta** deals with modeling and optimization of dynamic biological systems that are based on cellular models. Such systems are large-scale extensions of MPECs. Moreover, they have interesting modeling features since state dependent constraint functions with discontinuities also need to be treated through MPEC formulations. Moreover, **Brian Baumrucker** is currently considering the development of good MPEC formulations that model discrete decisions. He is currently working with the ROMeo real-time optimization package and is exploring 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. This work was presented at the annual AIChE meeting and a paper that describes this approach will appear in the next newsletter. In addition to the ROMeo comparison described above, he is investigating complementarity formulations in distillation columns with mass transfer limitation.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Researchers: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
 Shivakumar Kameswaran (Ph. D. completed August, 2006)
 Victor Zavala (Ph.D. started Fall, 2004)
 Yi-dong Lang (Jiansu Research Institute, Nanjing, China)
 Euclides Almeida Neto (Petrobrás, Rio de Janeiro, Brazil)

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. It can occur in open-loop unstable systems that arise in optimal control and nonlinear MPC, dynamic parameter estimation and the optimization of runaway reactors. Prof. Antonio Flores, a research colleague from the University of Iberoamericana, has demonstrated the advantages of this approach on a number of challenging polymerization processes. Moreover, the following research projects are currently being addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization, one based on reduced space and one on full space. First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called *DynoPC*. Written for Windows with a Visual Basic user interface and with heavy integration of graphical, simulation and automatic differentiation tools, this software package incorporates our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from <http://coin-or.org>. Current developments with *DynoPC* include ESO interfaces that are compliant with recently developed CAPE-Open protocols. This leads to an interface compatible with a number of existing process models and modeling environments. Since the last newsletter, **Euclides Almeida** has joined our group as a visitor from Petrobras. He is currently working on combining the EMSO interface, a modeling interface similar to gPROMS, with *DynoPC*. Moreover, the resulting package will be used to solve challenging industrial problems in dynamic optimization.

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. We are currently adopting a MATLAB framework and have coupled it with the AMPL modeling language. Domain specific prototypes have already been developed and work very well.

Consistency and Convergence of Simultaneous NLP Formulations for Dynamic Optimization

Does the solution of the discretized NLP converge to the solution of the original optimal control problem? What are the particular problem classes and assumptions for which this can be shown? This has been an interesting and long-standing research problem. Back in 1989, we have developed some consistency results based on the work of Reddien (1976) for Gauss collocation schemes. In addition, Lagrange multipliers from the KKT conditions have a direct relationship to adjoint variables from the Euler-Lagrange equations. However, more powerful convergence results are difficult to show and usually apply only to well-conditioned linear-quadratic control problems. Nevertheless, despite limited convergence results, very good performance is usually obtained with simultaneous optimization strategies.

Recently, Shiva has revisited some of the theory in order to derive properties for Radau and Lobatto collocation. Both of these methods (while of lower order) tend to behave much better than Gauss collocation. We have recently derived order conditions for these methods and have related their convergence properties to the more general class of boundary value solvers. Moreover, these have been verified by a number of example problems. Shiva has also extended this approach to problems with final time constraints. These properties are discussed in a reprint listed below.

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 advances 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 a project funded by ExxonMobil Chemicals, **Victor Zavala** has begun to develop multi-stage dynamic

optimization problems for grade transition and defouling 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. This approach is described in a reprint listed below.

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. This was described in a paper presented at the AIChE meeting where 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. This approach is demonstrated on a large-scale polymer process, where on-line calculation effort is reduced by over two orders of magnitude. 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 is described in the paper below. Finally, we have been developing a general Lyapunov-type stability analysis for this approach. This will be described in the next newsletter.

Finally, through collaborations with D. Subramanian and T. Samad at Honeywell, Inc. Arvind Raghunathan had been pursuing an important research problem on conflict resolution of aircraft trajectories. Given a set of aircraft with starting points, destinations, protection zones and obstacles, what are the optimal trajectories that lead to the best performance or minimum fuel consumption? Moreover, detailed flight models are employed that limit the maneuverability of these aircraft. This problem leads to a nonconvex dynamic optimization problem. Moreover, protection zones lead to disjunctive constraints that have been modeled through convex hull formulations. The resulting problems are discretized using collocation on finite elements and solved using IPOPT. More recently, **Juan Arrieta** has also extended this approach to a number of more complicated aerospace models including satellite trajectories and NMPC variations of these trajectories. His recent work has shown that our approach generates optimal solutions significantly faster than competing methods.

Large-Scale Optimization for Fuel Cell Models

Researchers: **Cong Xu (Ph.D. completed Spring, 2005, joint with Prof. M. S. Jhon)**
 Shivakumar Kameswaran (Ph. D. completed August, 2006)
 Parag Jain (Ph.D. started Fall, 2005)

Cong Xu recently completed his PhD and is doing postdoctoral studies. For his thesis project, he has been investigating 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, Cong Xu and Peter Follmann 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. These systems have been modeled and optimized with a variety of FORTRAN, MATLAB and MAPLE-based tools, such as OCC. 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. Finally, Parag Jain has begun to extend previous modeling and optimization work for Direct

Methanol 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. In the future, we expect this effort to be validated through experimental facilities at the University of Connecticut.

Reduced Order Models for PDE-based Units in Power Plant Flowsheets

Researcher: Yi-dong Lang (Jiansu Research Institute, Nanjing, China)

Student: Anshul Agarwal (Ph.D. started Fall, 2005)

Process simulation has become an essential capability that spans most tasks in process engineering, design and analysis. Simulation programs such as Aspen Plus, Pro/II and HYSYS are integrated into core engineering design activities. However, due to computational limitations, current process simulators usually deal with lumped parameter models that often do not capture detailed spatial characteristics of process units, including fluid flow and transport processes. As a result, they can suffer accuracy limitations and the loss of predictive capability. To overcome this difficulty, we are working with NETL on the Advanced Process Engineering Co-Simulation (APECS) project. Within this framework, process flowsheeting models (in Aspen Plus) have been successfully combined with computational fluid dynamics (CFD) models (using Fluent) to model multiphase systems, such as gasifiers and turbines within power plants. Current efforts are also focused on the inclusion of other distributed parameter custom models. In particular, an important, and challenging, application for this activity is the FutureGen Cycle, a 275 MW coal-fired power plant that includes hydrogen generation and CO₂ recovery, and requires multi-phase, spatially distributed models within its simulation environment.

To extend these NETL activities, we are developing and applying integrated optimization strategies that provide powerful tools for model development and process improvement. So far, these optimization problems are small-scale and efficient, and robust optimization algorithms are available that can be implemented easily. These features have led to the relatively easy and widespread adoption of optimization strategies. On the other hand, optimization strategies for CFD and distributed parameter models have seen far less development and this currently represents an important and challenging research activity. For APECS, which incorporates these models, we believe that optimization strategies will perform a key role in the development of advanced energy processes, such as the FutureGen Cycle. To provide a vehicle for the research tasks in this project, we consider the model components of the FutureGen Cycle flowsheet. This process includes a number of unit operations for coal gasification and byproduct (e.g., ash/slag and sulfur) separation; multiphase CFD models are needed for this purpose. Yi-dong Lang has been working with colleagues at Fluent Corp. to develop reduced order CFD models based on Proper Orthogonal Decomposition. This approach allows for a tremendous reduction in computing effort for the process flowsheet.

Moreover, feeding the gasifier with oxygen is an air separation unit (ASU) that is a significant energy consumer that must be optimized. Further downstream, 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 also require custom reduced order models. Anshul Agarwal has begun to develop reduced order models for these units as well using a novel space-time discretization.

Optimization and Control of Periodic Adsorption Processes

Student: Yoshi Kawajiri (Ph.D. started Fall, 2003)

Simulated Moving Bed (SMB) chromatography was developed in the 1960s as a realization of continuous chromatographic separation. Since then, SMB has been gaining attention in food, sugar, and petrochemical applications. In more recent years, SMB has been recognized as an attractive technology for enantiomeric separations in the pharmaceutical industry. An SMB system is realized by connecting multiple columns in a cycle. The feed and desorbent are supplied continuously between columns, and at the same time extract and raffinate products are withdrawn. Counter-current operation is “simulated” by switching these inlet and outlet streams intermittently in the direction of the liquid flow. As with PSA this system is characterized by a Cyclic Steady State

(CSS), where the concentration profiles in the columns change dynamically but repeat the same pattern in every cycle.

Over the past three years, **Yoshi Kawajiri** has been investigating efficient optimization strategies for these systems. Here optimization methods can be based on the single-discretization approach to discretize the Partial Differential Equations (PDEs) only in the spatial domain and then integrate the resulting Differential Algebraic Equations (DAEs) in time. On the other hand, the full-discretization approach discretizes the PDE both in time and spatial domain, leading to a large-scale Nonlinear Programming (NLP) problem. Yoshi has compared both approaches and found that the latter approach has shown tremendous improvements in the productivity of SMB systems. Moreover, these were obtained almost two orders of magnitude faster than with the single discretization (sequential) method used in gProms. The approach was applied to optimization of SMB systems with steady and time-varying feeds (i.e., PowerFeed), both for linear and nonlinear isotherms. This efficient approach also allows us to consider the design and control much more complex SMB systems. In particular, Yoshi has developed two superstructure SMB systems, one for a single step and the second over a full cycle, that allow for the optimization of a number of novel, recently reported designs, as well as some new ones. These superstructures lead to well-defined and easily solved problem formulations and lead to innovative designs with improvements in productivity. Moreover, through the formulation and solution of multi-objective optimization problems, we confirm that our approach has the potential to find more advantageous operating schemes than the standard SMB or PowerFeed operating schemes. These are described in two reprints listed below. Finally, we also show that these multi-objective solutions can be related to a class of profit maximization problems for SMBs. This is described in the paper listed below.

Ignacio Grossmann's Group

Open-Source Code for MINLP Optimization

New developments: **Open source code *bonmin* is now available in COIN-OR**

Post-doctoral fellow: **Pietro Belotti (Tepper)**

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

This project has been a collaboration with researchers at IBM (Andreas Wächter, Andy Conn, Joantahn Lee, Andrea Lodi). The main objective has been to develop open source code for solving MINLP problems.

The project has been initially restricted to MINLP problems that have a convex relaxation. The postdoctoral fellow Pierre Bonami, who has joined IBM, developed the code *bonmin* that solves MINLP problems with the NLP-based branch and bound, outer-approximation and the LP/NLP based branch and bound method. Both the outer-approximation and the LP/NLP based branch and bound method are based on our previous work (Duran and Grossmann, 1986; Quesada and Grossmann, 1992). The implementation provides a single computational framework for the three methods. The LP/NLP based branch and bound has been extended to a more general branch and cut scheme in which NLP subproblems do not have to be solved at only integer feasible nodes, but they can be solved at any intermediate node. For convenience we have termed this method “hybrid.” The code makes use of the following open source codes: IPOT from Andreas Wächter and Larry Biegler, and CLP or CPB from the COIN-OR library.

Pierre has extensively tested his code with close to two hundred test problems that Nick largely helped to build. These include batch design, retrofit planning, layout and trim loss problems. Carl Laird also contributed with some water contamination problems that involve a large number of continuous variables. The test problems are available in the webpage: <http://egon.cheme.cmu.edu/ibm/page.htm> The performance of the open source code was compared with both SBB, the branch and bound code in GAMS, and DICOPT, the outer-approximation method that is also available in DICOPT. On a representative subset of 38 of the 200 problems showed the following trends. DICOPT solved 20 of the 38 problems the fastest and in less than 3minutes. The hybrid method (i.e. branch and cut) proved to dominate for the remaining 18 problems in terms of speed and successful completion. The hybrid method always dominated the NLP-based branch and bound as well as the open-source outer-approximation method.

With the addition of Pietro Belotti, our next major step in this project will be to extend the code for handling nonconvexities, both with a non-rigorous approach, as well as with deterministic global optimization approaches that rely on the use of convex envelopes..

Algorithms for Nonlinear Disjunctive Programming

Student: Nicolas Sawaya [Ph.D., to complete end of Aug 06]
Research collaborator: Aldo Vecchietti [Researcher at INGAR]
New Developments: Theoretical connection established between GDP-Balas' disjunctive programming
 New framework for derivation of stronger relaxations

Nicolas Sawaya

Nick defended his Ph.D. thesis in November and joined ExxonMobil, Corporate Research. His work ended with a truly high note. The initial objective of Nick's project has been to develop novel solution methods for generalized disjunctive programs (GDP), in particular effective cutting plane methods for linear GDP problems. The second objective was to find effective ways of solving nonlinear GDP problems using the convex hull reformulation. The final objective was to establish a theoretical connection between GDP and disjunctive programming, which led to the surprising discovery that it is possible to obtain stronger relaxations than the one based on the convex hull formulation by Lee and Grossmann.

The first step in Nick's research work was to develop a solution method for linear GDP problems that relies on cutting planes, and that can be embedded within a branch and cut algorithm. The major steps of the algorithm are to first solve the big-M relaxation. Next, a separation problem is solved in which the difference is minimized between a feasible point in the convex hull relaxation and the solution of the big-M problem. Here the 1, 2 or infinity norm can be used, with the first and last leading to linear objectives. If the difference in the separation problem is small or even zero this is a clear indication that the both the big-M and the convex hull relaxations are essentially identical. If, on the other hand, the difference is not small one can derive a cutting plane. The derivation of successive cutting planes continues until the improvement in the lower bound of the big-M model lies within a tolerance. The idea is then to switch to a branch and bound method. Nick applied his cutting plane technique with the infinity norm to the strip packing problem that consists of fitting a set of rectangles in a roll of fixed width in order to minimize its length. The proposed cutting plane method led to order of magnitude reductions in the CPU time compared to both the big-M and convex hull formulation. Nick also solved a 10 process retrofit problem, and a job-shop scheduling problem. The cutting plane technique was not very helpful in both cases, although in the retrofit problem it did improve substantially the performance of the big-M reformulation. Nick also been investigated the use of cutting planes for solving nonlinear disjunctive problems. Nick tested this method on a retrofit planning problem, where he obtained 50% reduction in CPU time.

In the application of the convex hull, and important question is how to implement the constraint $\lambda g(v/\lambda) \leq 0$ for the case when λ goes to zero and when g is nonlinear and convex. In our previous work we had used the approximation $(\lambda + \varepsilon) g(v/(\lambda + \varepsilon)) \leq 0$, which can give rise to problems depending on how ε is selected. If ε is set too small there are difficulties with accuracy. If ε is somewhat large then if a disjunctive term does not apply and the inequalities are violated, it may make the approximation infeasible. Nick showed that a rigorous approximation that avoids both problems is given by $(\lambda_{jk} + \varepsilon) g_{jk}(v_{jk}/(\lambda_{jk} + \varepsilon)) \leq \max_{v_{jk} \in (0, U_{jk})} (\max(\varepsilon g_{jk}(v_{jk}/\varepsilon), \varepsilon g_{jk}(v_{jk}/(1 + \varepsilon))))$, where the basic idea is that the term on the right hand side represents a relaxation that can be made arbitrarily small. Since the constraints are convex, the maximization on the right hand side can be computed by evaluating the functions at the extreme points for each inequality which are few for sparse problems. In this way the actual expression can be simplified to, $(\lambda_{jk} + \varepsilon) g_{jk}(v_{jk}/(\lambda_{jk} + \varepsilon)) \leq \max(\varepsilon g_{jk}(0), \max_{v_{jk} \in (0, U_{jk})} \varepsilon g_{jk}(v_{jk}/(1 + \varepsilon)))$. Nick also found an alternative expression given by $(\lambda_{jk} + \varepsilon)(g_{jk}(v_{jk}/(\lambda_{jk} + \varepsilon)) + g_{jk}(0)(\lambda_{jk} - 1)) \leq 0$, which is easier to implement. Nick was able to show that the latter expression is superior compared to the first one in terms of accuracy, under most circumstances. The exceptions rarely hold true. Nick has successfully tested this approximation scheme in several examples (analytical, process network, safety layout) using values of $10^{-7} \leq \varepsilon \leq 10^{-4}$. The results have shown that very good approximations are obtained with both methods. Furthermore, based on input by Kevin Furman from ExxonMobil, Nick considered the

alternative convex expression $((1-\varepsilon)\lambda_{jk} + \varepsilon)g_{jk}(v_{jk}/((1-\varepsilon)\lambda_{jk} + \varepsilon)) - \varepsilon g_{jk}(0)(1-\lambda_{jk}) \leq 0$ which not only circumvents the infeasibility that arises in the original Grossmann & Lee expression, but, when $0 < \varepsilon < 1$, it is exactly equivalent to the (true) CH expression at $\lambda = 0$ or 1 , regardless of the value of ε within that range. Nick has numerically tested the various schemes concluding that the Furman approach seems to work best.

In the last part of his Ph.D. thesis Nick studied in great detail the pioneering papers by Egon Balas on disjunctive programming. In doing so, he was able to establish a nice theoretical connection between the generalized disjunctive programming (GDP) model that we have been considering and the disjunctive model by Balas. This is non-trivial because the major difference is that the GDP model includes Boolean variables for establishing the truth of the disjunctions and logic relations between the discrete decisions. The major point that emerged from Nick's analysis is that if we formulate the linear GDP problem by explicitly adding the OR constraint on the Boolean variables,

$$\begin{aligned}
 \text{Min } Z &= \sum_{k \in K} c_k + d^T x \\
 \text{s.t. } & Bx \geq b \\
 & \bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk} x \geq a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K \\
 & \bigvee_{j \in J_k} Y_{jk} \quad k \in K \\
 & \Omega(Y) = \text{True} \\
 & x^L \leq x \leq x^U \\
 & Y_{jk} \in \{\text{True}, \text{False}\} \quad j \in J_k, k \in K \\
 & c_k \in \mathbf{R}^1 \quad k \in K
 \end{aligned}$$

then if we define the continuous variable λ_{jk} to represent the Boolean variable Y_{jk} , and convert the logic constraints into inequalities, the following formulation can be obtained:

$$\begin{aligned}
 \text{Min } Z &= \sum_{k \in K} c_k + d^T x \\
 \text{s.t. } & Bx \geq b \\
 & \bigvee_{j \in J_k} \begin{bmatrix} \lambda_{jk} = 1 \\ A^{jk} x \geq a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K \\
 & \sum_{j \in J_k} \lambda_{jk} = 1 \quad k \in K \\
 & H\lambda \geq h \\
 & x^L \leq x \leq x^U \\
 & 0 \leq \lambda_{jk} \leq 1 \quad j \in J_k, k \in K \\
 & c_k \in \mathbf{R}^1 \quad k \in K
 \end{aligned}$$

The above model corresponds to a continuous disjunctive program in an intermediary form between its disjunctive and conjunctive normal forms in which the integrality of the variables λ_{jk} is guaranteed. Having this formulation establishes a direct link with Balas' work where one can then apply the wealth of theoretical results that he has developed. Among these, a major result is to realize that the convex-hull model by Lee and Grossmann is part of a larger family of MIP reformulations. These depend ultimately on the number of basic steps that are applied from conjunctive to disjunctive normal form. To use simple words, what it means is that by intersecting constraints within the disjunctions, one can obtain stronger relaxations.

Nick has illustrated this first with a small network problem, in which the recursive intersection of disjunctions yields a single disjunction where each term corresponds to one structural alternative in the topology. He has also illustrated this with strip packing problems involving 4, 25 and 31 rectangles. By intersecting disjunctions corresponding to the largest “bottleneck rectangles” he could solve the 4 rectangle problem as an LP! In the 25 rectangle problem the lower bound was increased from 9 (convex hull) up to 27, with 31 being the optimal solution. In the 31 rectangle problem the lower bound was increased from 10.64 up to 33, with 33 being the optimal solution. Needless to say, these results are truly exciting.

Nick will be completing his papers in the next couple months in which he can also in a very elegant way show that his infinity norm cutting plane is equivalent to the 1-norm of the dual of the reverse polar formulation by Balas. These papers will undoubtedly represent a major step in the area of disjunctive programming. The new student Juan Ruiz will be the next student in line who will work in this project.

Aldo Vecchietti: LOGMIP and DICOPT

Aldo and his students at INGAR in Argentina are developing the LogMIP code, which is as 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 implemented LogMIP in the IDE version of GAMS and tested it with several problems. Aldo has also automated the logic-based OA algorithm by Metin Turkay, which is suitable for nonlinear GDP process network problems. Work in collaboration with GAMS, using Nick’s transformations, is under way to implement the reformulations for nonlinear GDPs. The LogMIP Website provides the possibility of downloading the code: <http://www.ceride.gov.ar/logmip/>. The Website also includes now some explanation about LogMIP, the User’s manual, solvers and examples downloads, references and links.

Aldo has recently added a capability in DICOPT for handling more effectively infeasible NLP subproblems. What Aldo has done is to allow the addition of linearizations of the infeasible NLP subproblems. This option is rigorous for the case of convex MINLP problems. For nonconvex problems there is the risk of cutting off optimal solutions. To solve problems in GAMS with linearization in infeasible NLPs the following option must be defined: infeasder 1. By default infeasder is 0. In this case DICOPT runs like the previous version (just with the integer cut with NO linearization on the infeasible points). This new option has shown to significantly improve the performance of DICOPT in several problems, which often did not converge with the old version. This performance has also been verified by Nick Sawaya on several difficult layout problems that tend to produce infeasible NLP subproblems.

Global Optimization of Integrated Process Water Systems

New developments: **Completed paper on multiscenario optimization of water systems under uncertainty**

Students: **Ramkumar Karuppiyah [Ph.D. started Jan 04]**

Visitor: **Eugenio Bringas (Univ. Cantabria, Spain, Sept-Dec 05).**

Ram’s project has dealt with the global optimization for the synthesis of process water systems that integrate the water reuse section for processes with the distributed water treatment section for a given number of pollutants. The initial objective has been to find for given sets of processes and given treatment units the optimal configuration of the system that minimizes the use of freshwater, or more generally that minimizes the total cost. Ram has assumed for the processes units that they are either characterized by fixed contaminant loads, or by variable loads that obey mass exchange constraints in terms of concentrations. For the treatment units fixed recoveries are specified. Ram

has considered the extension to synthesis for multiple scenarios in order to handle uncertainties in the contaminant loads and recoveries in the treatment units. This work he has generalized to generic multiscenario problems.

For the synthesis of the integrated water system, Ram developed a superstructure that involves for a given number of process units and treatment units all possible alternatives for interconnection of process and treatment units, and mixing and splitting of streams. The model corresponds to an NLP model with bilinearities in the mixers given by the product of flows times concentrations in ppm of the contaminants. Ram developed a global optimization algorithm that relies on combining spatial branch and bound search, with piecewise linear approximations inspired by the work of Lorena Bergamini. The motivation is that piecewise linearizations improve the quality of the lower bound, but they do it at the expense of introducing additional 0-1 variables. For this reason it is sensible to still use a spatial branch and bound search, but strengthened by piecewise linearizations for a fixed (modest) number of intervals. To also strengthen the quality of the lower bound, Ram has derived a valid cut that represents overall mass balances for each of the contaminants. This cut has proved to be extremely effective. The algorithm also relies on bound tightening and on branching only on the flows. The bisection rule is used for partitioning. Ram has tested his method with several examples. In one problem involving 4 process units and 3 treatment units the NLP had 195 variables and 151 constraints. CONOPT either did not converge, or if it did, the best it found was 186.18 ton/hr. Our proposed method converged to the global optimum of 170.39 ton/hr, requiring only 10.3 secs solving the problem at the root node. BARON in contrast required 3490.5 seconds and 9656 nodes. When the valid cut was added to BARON, the computing time was also reduced drastically. Ram has extended the model to general cost functions and selection of treatment units, which gives rise to an MINLP model due to 0-1 variables that are needed to model these units.

As a next step in his research, Ram has considered the extension of the above problem to the case when the water system must operate under multiple scenarios in which the loads in the units as well as the recoveries in the treatment units are uncertain, and therefore change in each scenario. This problem gives rise to a two-stage stochastic programming problem. The first stage costs include the investment cost for piping which depends on the maximum flowrate allowable in a pipe, and the design cost of each treatment unit, which is dependent on the maximum flow of wastewater handled by that treatment unit. The operating costs of the network appear in the second stage, which include the cost of obtaining freshwater for use in the process units, the cost of pumping a certain flow of water through the pipes and the operating costs in the treatment units. The difficulty of the global optimization for the nonconvex multiscenario problem is that the corresponding NLP or MINLP becomes much larger. Furthermore, 0-1 variables must be introduced for the piping in order to control the potential complexity in the configurations for each period. Ram developed a solution method that is based on a branch and cut algorithm. The basic idea consists in performing a spatial branch and bound where cuts are generated at each node using a Lagrangean decomposition scheme. These cuts are obtained by globally optimizing each scenario independently. These cuts are then added to the original problem that is convexified by constructing convex envelopes for the non-convex nonlinear terms leading to an MILP that is solved to predict a rigorous lower bound to the global optimum. A heuristic is used for the generation of good upper bounds. These lower and upper bounds are converged within a specified tolerance in a spatial branch and bound algorithm. Ram considered a problem with 2 process units and 2 treatment units and 10 scenarios. The MINLP model involved 28 binary variables, 868 continuous variables, 1044 constraints and 490 non-convex terms. The application of the proposed algorithm yields an expected cost of \$651,653.06, which is the global solution to the problem. The lower and upper bounds converge within 1% tolerance at the root node of the branch and bound tree. The proposed algorithm takes a total of 62.8 CPU secs to solve while BARON could not verify optimality of the upper bound after 10 hours of CPU time. Ram was able to generalize the above cited branch and cut algorithm for generic multiscenario problems, which was submitted for publication.

Eugenio Bringas

The aim of the work by Eugenio, which was conducted in collaboration with Ramkumar, was to obtain the globally optimal design of an emulsion pertraction plant, that consists of a prespecified number of hollow fiber modules (MOD), mixers (MU) and splitters (SU), with various possible interconnections between the units. The specific objective of this work has been to identify the interconnections of the superstructure and the flowrates and the contaminant compositions of the streams, such that we meet the discharge composition regulations using a minimum area of the membranes. In order to address this problem, Eugenio proposed a superstructure for the aqueous feed solution and the emulsion stream which flow counter currently inside a hollow fiber module where the transfer of contaminant takes place between the aqueous phase and the emulsion phase. In the postulated structure, the aqueous

phase flows continuously, while the emulsion phase operates in batch mode. To solve the associated superstructure optimization problem, Eugenio and Ram developed a two-stage approach in which a simplified version of the model is first solved to rigorous global optimality. In a second stage the rigorous model is solved by using as a starting point the solution of the problem in the first stage. The global optimization algorithm relies on a spatial branch and bound algorithm in which tight lower bounds on the global optimum are generated through cuts obtained from Lagrangean decomposition, similar to the work of Ram for multiscenario optimization. The only difference is that in this case the Lagrangean relaxation is decomposed into two subproblems pertaining to the aqueous phase and to the stripping phase which are optimized independently for fixed values of the multipliers. Eugenio applied this technique to a system consisting of 2, 3 and 4 membrane modules. As one might expect the proposed method becomes more competitive as the size of the problem increases.

Optimal Design of Corn-based Ethanol Plants

New developments: **65% reduction in steam consumption; 11% reduction in manufacturing cost**

Students: **Ramkumar Karuppiah [Ph.D. started Jan 04]**

Visitor: **Mariano Martin (Salamanca), Andreas Peschel (RWTH Aachen)**

This project was initiated with the exchange student Andreas Peschel and Ramkumar Karuppiah in collaboration with Cargill. Mariano Martin has continued recent work with the help of Ramkumar. The objective has been two-fold: a) Develop short-cut models for corn-based ethanol plants; (b) Develop a superstructure optimization model to determine the extent to which the design of these plants can be improved.

In the first phase of this work, a simplified model was developed for the “dry-grind” process for the corn-based bio-ethanol plant. In such plants, fuel ethanol is produced using corn-kernels as the feedstock. Fuel grade ethanol has to be 100 % pure before it can be blended with gasoline to be used in automobiles. However, conventional distillation columns produce an azeotropic mixture of ethanol and water (95 % ethanol – 5 % water), which has to be purified further for making fuel ethanol. The main challenge in the way of producing fuel ethanol commercially is that the process is very energy intensive and requires large amounts of steam and electricity for use in the rectifiers to get an azeotropic mixture of ethanol and water and requires the use of expensive molecular sieves to get 100 % pure ethanol. Furthermore, the waste spillage from the fermentation units, which is rich in volatile organic compounds, and the other wastewater streams in the plant have to be treated before disposal, which, in turn requires energy intensive units like centrifuges and dryers. Due to the high costs involved in this process, currently it is not economically feasible to produce fuel ethanol commercially and sell it in the open market without subsidies. If the economics of the process have to be improved, we would need use process synthesis tools similar to those being used in the petrochemical industry to design optimally operating plants, rather than use ad-hoc or empirical approaches to build such systems. We look at the problem in a way to reduce the operating costs of the plant and minimize the energy usage and maximize the yields of the plant.

In order to design such a bio-ethanol plant, Andreas, and Ram initially developed a model to predict the performance of the flowsheet that includes grinding, scarification, fermentation, centrifugation and drying operations. A superstructure was also postulated in which some of the major alternatives include separation by molecular sieves and or corn grits, and different ways to accomplish the drying for the dried grains solids, the cattle feed by-product. The process units are interconnected to each other through network feed flows and other utility streams. The objective is to optimize the structure, determining the connections in the network and the flow in each stream in the network, such that we minimize the energy requirement of the overall plant while trying to maximize the yields. The optimization without heat integration (MINLP model) led to a decrease of the manufacturing cost from \$1.61/gal (base case) to \$1.57. In the next step heat integration was considered in the optimization, which further reduced the cost to \$1.51/gal. However, it became clear that the scope of heat integration is limited by the relatively low temperature in the fermentor. In order to improve the potential for heat integration we considered multi-effect distillation in the “beer” column and in the azeotropic column as alternatives for the optimization. This finally, led to a 65% savings in steam consumption and cost reduction down to \$1.43/gal.

In this way, the production of “bio-ethanol” along with other co-products and commodities in a bio-refinery using biomass as a sustainable source of fuels is significantly improved in terms of the economics and energy efficiency.

These results are highly significant because most of the current work has been aimed at improving the yield in the fermentation reaction, and to our knowledge savings of this magnitude have not been reported for the separation part of the process.

MINLP Flowsheet Optimization with Process Simulators

New developments: **New paper that describes use of simulators in MINLP flowsheet optimization**

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

While most of the work with Jose Caballero has concentrated on thermally integrated separation sequences, one additional piece of work has been the incorporation of process simulators for MINLP optimization in process flowsheets.

A major motivation for the work has been that in Process Synthesis, GDP and MINLP models are limited to moderated size problems. The reasons are that the number of equations implied in chemical process models can be very large with hundreds or even thousands of integer (binary, Boolean) variables and with a large number of nonlinear and nonconvex equations that can prevent not only to finding the optimal solution but even finding a feasible point. Also, a rigorous modeling approach requires the use of process simulators that include state of the art models. Although most process simulators have optimization capabilities, they are able to deal only with problems involving continuous variables and smooth constraints with continuous domains. Therefore, complex cost models or detailed sizing models included in some simulators cannot be used. For this reason Jose has investigated different algorithms to integrate GDP and MINLP algorithms with existing process simulators in order to include complex cost and/or size functions, or in general complex equations defined over discontinuous domains. These functions can be in the form of explicit equations or implicit blocks (input-output black box relations). The structural optimization of process flowsheets (topology optimization) will be addressed at a later stage.

Jose has investigated three different algorithms using an MINLP reformulation of the original disjunctive problem: BB, OA and LP/NLP-BB. The basic idea relies on working in the reduced space of the decision and convergence variables in order to define the linearization in the MILP master problem. The bottleneck of all the procedure is in the time spent by the NLP that is related mainly to the time used in estimating accurate derivatives. The public version of HYSYS.Plant was used and the NLP subproblems were solved using CONOPT and SNOPT (external to HYSYS) through an activeX client-server application. All the process is controlled by MATLAB . Cost and size models were also developed in MATLAB as third party implicit models or through explicit equations. Jose was able to solve several problems including discontinuous costs in heat exchanger networks and natural gas plant, equipment choices in di-methyl ether plant. The problems were all solved with reasonable computational times (about 2,000 CPU sec largest problem). Jose found that the size of the master problem using implicit equations is greatly reduced in comparison with an equation oriented approach. Also, relaxing blocks of equations, instead of each equation individually, (i.e. by a big M reformulation) seemed to produce better relaxation gaps. The paper describing this work is listed in the section on references.

Synthesis of Crystallization Processes

New developments: **New aggregated model for superstructure optimization**

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

Motivated by a project we had with BP for the separation of Para-Xylene with crystallization, Ricardo, the new postdoc from Porto in Portugal, has considered the generalization of that work for the superstructure optimization and study an effective solution method for the associated MINLP problem. As a first step he simply considered the simultaneous solution of the MINLP and found, as Carlos Mendez had, that it is extremely difficult to converge the problem, mostly because the NLPs become infeasible. Therefore, the major approach that Ricardo has taken is to consider a two-level decomposition consisting of the solution of an aggregated and a detailed model. The key idea in

the aggregated model is to merge the units in crystallization and centrifuge blocks as a single input-output block so that the aggregated model is defined in the space of interconnection of major blocks so as to determine for instance the number of crystallization stages. Once an alternative is selected by the aggregated model the detailed model considers superstructures for the crystallizers or centrifuges in the selected blocks. Ricardo has tested independently the solution of the aggregated and detailed model with fixed choices and found that the MINLP

Design for Sustainability

Post-doctoral fellow: Gonzalo Guillen

This is a new project in which Gonzalo, a postdoc with a Fulbright fellowship, is trying to incorporate sustainability considerations in the synthesis and design of chemical processes. The final aim is to provide a set of quantitative tools based on mixed-integer modeling techniques that will allow the computation of the set of efficient solutions, in terms of economic benefit and environmental impact, for a wide range of problems arising in PSE. These solutions should then be used by the decision-makers to choose the best ones according to their preferences and taking also into account the applicable environmental rules and legislation.

As a first step, Gonzalo has studied different ways of incorporating environmental concerns into the existing mathematical formulations developed for diverse PSE problems. As a result of this preliminary step, the Eco-indicator 99 has been chosen, among other metrics available in the literature, as the most appropriate environmental impact measure to be appended to the objective function. The Eco-indicator 99 reflects the newest advances in the damaged oriented method recently developed for Life Cycle Assessment (LCA) and it proposes 11 impact categories that can be further classified into 3 specific damage categories, namely human health, ecosystem quality and resources. The selection of this approach has been motivated by its holistic view of the system, as it covers the entire life cycle of the product, process or activity, encompassing extracting and processing of raw materials; manufacturing, transportation and distribution; reuse, maintenance; recycling and final disposal. This metric has been incorporated first in the MINLP superstructure optimization model applied to the hydrodealkylation process of toluene (HDA), a case study that was originally proposed by Douglas. The second formulation has been the long-range planning model of process networks. The predicted solutions show that a trade-off naturally exists between profit and environmental impact and that more sustainable decisions can be adopted if one is willing to compromise the economic benefit of the company. Furthermore, what has clearly emerged as a critical issue in both cases is the high level of uncertainty associated with the parameters involved in the computation of the Eco-indicator 99. Thus, Gonzalo is currently studying different ways to address this issue. Specifically, he is assessing the use of stochastic mathematical programming techniques as a way to control the variability of the environmental impact and maximize at the same time the economic benefit of the process.

Design and Planning of Deep-Water Oilfield Development under Uncertainty

New Developments: Formulation of MINLP model and preliminary solution method

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

The project of Bora Tarhan, who recently presented his Ph.D. proposal, follows the line of work of Vikas Goel for the design and planning of gas and oil fields under uncertainty. As a first step Bora has addressed a different stochastic optimization problem that in principle is simpler to model in order to prepare the ground for the complex gas and oil field problem. The problem is as follows. A network of candidate processes is given over a specified time horizon that is described by multiple time periods in which product demands are specified. It is assumed that major uncertainties are involved in the yields of each process, which are described by probability distribution functions. We consider that 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, it is assumed that 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 in making planning decisions for process selection, capacity expansions, and possible investment in pilot plants in order to maximize the expected net present value over the specified time horizon.

In order to capture all the complex trade-offs, Bora developed a new mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints that are similar in spirit to Vikas's model. One importance difference is the time varying uncertainty, which for simplicity Bora considered is revealed over two time periods. Furthermore, he assumed that the time required for a pilot plant study corresponds to one time period, meaning that uncertainty is reduced to only one time period. This scheme is quite restrictive but we adopted it as a simplifying assumption that we intend to relax at a later stage. In order to solve this special multi-stage stochastic program Bora initially reformulated it as an MILP, which can be solved through an LP-based branch and bound. However, this approach is restricted to smaller instances. Therefore, Bora has developed a dual Lagrangean branch and bound method, also similar in spirit to the work by Vikas Goel. The corresponding subproblems are obtained by relaxing the disjunctions and transferring the first period non-anticipativity constraints to the objective function with Lagrange multipliers. The resulting model can be rewritten as independent subproblems for each scenario. The overall objective is to find the minimum upper bound by updating the multipliers. The branch and bound involves branching over both discrete and continuous variables that are involved in the non-anticipativity constraints. Bora has successfully applied this method to a small 3 process network, with one existing process and two with new technologies and for which investment of pilot plants can be considered over a 10 year horizon. Reformulating this problem as a single MILP involves 7,360 0-1 variables, 8,841 continuous variables and 85,139 constraints. Using CPLEX after one week the best solution that could be obtained had a net present value of \$61.5 million. With the proposed method a solution of \$80.14 was found in 10 hours of CPU time with a gap of 3%. The proposed solution did not select pilot plants to reduce the uncertainty, and proposed expanding Process I up to a capacity of 10 tons/day and making an additional expansion of 4.49 tons/day at time period 1 if the yield turns out to be 69%. If the yield for Process I is found to be 81% then an expansion of 2.98 tons/day is made also at the time period 1. The manuscript on this work has been submitted for publication.

Bora spent his internship at ExxonMobil's Upstream Research Center in Houston to get acquainted with planning problems related to deep-water oilfield development. The problem he has considered is the one of an oil field consisting of a number of reservoirs where each contains several possible well sites. Some of these well sites have to be drilled and exploited for oil over a planning horizon. The oil field infrastructure can be composed of Floating Production Storage and Offloading (FPSO) and/or Tension Leg Platform (TLP) facilities. The FPSO facility can be either a small FPSO, converted from a retiring oil tanker, or a large FPSO, newly constructed grassroots facilities. An FPSO facility can produce, store and offload the produced oil to other tankers. Unlike FPSO, a TLP facility cannot produce oil; it possesses only drilling and oil recovering capability. TLP and FPSO facilities can be connected to each other through pipes. Each facility has a construction cost and a lead time between the construction decision and the actual start-up. There are two options for drilling wells. Each well can be drilled as a sub-sea or a 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. Unlike sub-sea wells, a TLP well has to be drilled by a TLP facility. In order to recover oil from a well, it must be connected to a facility. A sub-sea well has to be connected to an FPSO facility, whereas a TLP well has to be connected to a TLP facility. The problem then consists of selecting investment and operation decisions such as selection of the type, location of facilities, time to build them, selection of wells to drill, the time to drill each well, time to connect each well to the facilities and production from the wells. There are uncertainties in the sand quality, size of the reservoir and breakthrough time. Given the above assumptions, the goal is to maximize the expected net present value of the project. Bora has made several assumptions: strong aqueous support which creates enough pressure in the reservoir; no need for enhanced recovery, all wells in one reservoir are identical. Given the cumulative oil extracted from a reservoir, all wells in that reservoir have the same maximum oil rate. A simplified reservoir model has been considered where the oil rate decreases linearly, and the water-to-oil ratio is follows a nonlinear function with the cumulative oil production.

As a first step, Bora has developed an MINLP model in which facilities and wells of the original problem are aggregated. Instead of deciding which well to drill or which facility to build, the decisions are how many wells or facilities to build. Because of aggregation, variables for connection of facilities and wells are disregarded, and lengths to wells are underestimated in order to guarantee that the model predict an upper bound on the detailed model. This model is similar to the process networks model with the exception that each scenario is a non-convex MINLP. The steps of the algorithm are the same, except that each subproblem is solved using a global optimization algorithm. This relaxation yields an upper bound and the lower bound is generated by a simple heuristic. At this point Bora has only performed the subgradient iterations at the root node of the branch and bound tree to find a better upper bound. The best feasible solution is obtained on an example had an expected NPV of \$4.5x10⁹. In the optimal solution, the model predicts start building one TLP and three small FPSO facilities so they become ready at the beginning of years 2 and 3. After that, drilling of 6 TLP wells starts for five consecutive years. Also, 12 sub-sea

wells are drilled starting from the first year for three consecutive years. Bora should have completed the major part of the algorithm by the next newsletter.

Simultaneous Planning and Scheduling of Multiproduct Plants

New developments: **Development of novel aggregate planning model for parallel batch reactors**
 Extension of continuous multiproduct to case of parallel units

Students: **Muge Erdirik [Ph.D. started Jan 2004]**

Muge's project deals with the simultaneous planning and scheduling of multiproduct plants. The initial objective in her work has been to consider the case of a single processor on which a number of products must be produced continuously over a given number of time periods. Sequence-dependent changeovers are given and due dates are assumed to take place at the end of each time period. The objective is to determine a production plan and schedule in order to maximize the profit (income minus inventories and changeovers). She has also considered recently the extension to the case of parallel processors.

To address the scheduling problem described above, Muge first developed a detailed slot-based MILP scheduling model. This model cannot be used to solve planning problems that typically require long time horizons. A simple approach to circumvent this problem is to develop an aggregate planning model that does not include all details such as changeovers. Well-known limitations of such an approach are inconsistencies between planning and scheduling and loss of optimality. Therefore, our objective has been to develop an iterative scheme that relies on aggregated models but that is guaranteed to converge to the same solution as if we had solved the detailed scheduling model. In order to accomplish this objective Muge developed an aggregated MILP model that underestimates the changeover times and includes 0-1 variables for deciding what products may be produced in a detailed schedule. The iterative scheme consists in solving a sequence of aggregated MILP planning models and detailed scheduling models with fixed assignment of products to be produced at each time period. In addition to using a simple integer cut, Muge has developed superset, subset and capacity cuts that eliminate a larger number of alternatives. For the cases where the detailed scheduling model with fixed assignments can still be expensive to solve, we can resort to a rolling horizon solution approach. Muge has tested extensively her solution method. She considered two major cases: high lower bounds for the demands bound, low lower bounds for the demands. In a 24 week problem (720 0-1, 5907 continuous, 5526 constraints) the proposed method converged within 6% of the optimum in 3190 secs while the detailed model did not terminate the search after 4000 secs (18% gap of bounds) and obtained an inferior solution. In the case of low demand the proposed method converged in 8 secs within 4% of the optimum while the simultaneous approach did not terminate after 3000 secs. Muge has recently addressed the extension of this problem to the case of parallel units. The solution approach is similar except that the aggregate model has two new features: (a) sequencing constraints that provide a more accurate estimation of changeover (see Dow project below); (b) a more effective formulation of changeover constraints that is tighter and requires fewer constraints. We will report computational results on her work in the next newsletter.

Based on an internship at Dow Chemical in Midland, Muge has been addressing the simultaneous multisite planning and scheduling problem for batch reactors, a case study that was selected by Dow for the Enterprise-wide Optimization project. The specific problem is as follows. We are given a set of production sites, each with a unique set of raw material costs, raw material availability, storage tanks with associated capacity, transportation costs to each customer, reactors with associated materials it can produce and batch sizes and times for each material it can produce, as well as operating costs for each material, sequence dependent clean out times, and time the reactor is available during a given month. We are also given a set of customers, each with a unique set of demand and prices for desired product. Finally, specified are the materials produced: process intermediates and final products. Dedicated storage tanks are considered. Another issue is that a final product of one process may be used as a raw material for another process within the site. However, once a final product is fed to the dedicated storage tank, it can not be retrieved back to the plant. The problem is then to determine the monthly production quantities for each reactor and the assignment of materials to storage tanks to maximize profit.

Muge has considered first the case of a single site. For this she proposed a novel continuous time MILP optimization model for scheduling that is based on slot time representation that overcomes some of the major difficulties faced by

the STN and RTN discrete and continuous time models. While effective for short-term scheduling, the proposed model becomes computationally very expensive to solve for long planning horizons. Therefore, as in the case of the single continuous processor, Muge has devised a rigorous bi-level decomposition algorithm. The problem is decomposed into an aggregated upper level planning and a lower level planning and scheduling problem. The upper level determines the products to be produced at each time period as well as number of batches of each product, production levels and product inventories. The upper level is based on a new relaxed STN model where the detailed timing constraints and changeovers are replaced by time balances yielding a tight upper bound on the profit. A major new development here has been the *incorporation in the aggregate planning model of sequencing constraints* similar to the ones in the traveling salesman problem that yield accurate predictions for the changeovers. The lower level is solved in the reduced space of binary variables according to the information obtained from the upper level model; therefore it yields a lower bound on the profit. The lower level determines production and inventory levels as well as detailed timing of the sequence of products and associated assignments to processing equipments and storage tanks. The procedure iterates until the difference between the upper and lower bound is less than a specified tolerance. The proposed decomposition scheme ensures consistency between the two levels and optimality within a specified tolerance. The biggest surprise with the new aggregated model is that for small problems (e.g. 5 products, 2 reactors) it usually the exact scheduling solution (i.e. zero gap). For larger problems it predicts much smaller gaps than a relaxed model that simply underestimates the changeover times. A limitation, however, is that the new aggregate model leads to a larger MILP model. This, however, can be solved with a rolling horizon approach, with relatively small compromise of the optimality. As a specific example in a problem with 10 products and 5 reactors, over 24 week period, the problem involved 7,776 0-1 variables, 19,344 continuous variables, and 32,126 constraints and was solved in about 7,000 secs. Muge is currently preparing the manuscript on this work. Also, for future work will also look at the extension to multiple sites.

Design and Planning of Responsive Supply Chains

New Development: Models for planning and design.

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

The major goal of this project, which is being performed by Fengqi You 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 across the supply chain. The motivation for this project is that virtually all optimization models assume that material can be transferred instantaneously. In that way lead times, or response times once orders are placed, are not taken into account. It is our major goal to establish the trade-offs between economics and lead times.

As a first step Fengqi has addressed the long term design problem, for which he has developed a model for designing the supply chain of multisite network of processes in a superstructure that involves both dedicated and multiproduct continuous plants. The time horizons considered are of the order of years, and zero-inventory levels are considered, which qualitatively corresponds to the worst case for lead times. The problem is then posed as a bi-criterion optimization problem in which the objectives are to maximize net present value and to minimize lead time. In order to reflect lead times for different choices of topologies Fengqi has 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 times these are simply constants, while for multiproduct plants they correspond to cycle time plus residence time minus its processing time. Note that the cycle time results from a scheduling optimization that has to be accounted. For the case of dedicated plants the problem can be formulated as an MILP, since nonlinear terms defining the lead times can be linearized. For the case of multiproduct plants, the model and leads to a nonconvex MINLP problem. Fenqui has 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 located in PA, TX and AL. the PA site can install all the three types of plants, the TX sites can only install plant I, and the AL site can only install plant 2 & 3. Two suppliers of ethylene are located in TX and OH, and two suppliers of benzene are located in TX and VA. Two customers of SPS resins are located in CA and NY, another two customers of EPS resins are located in GA and MN. For 3 time periods (2, 3 and 5 years) the model involved 133 0-1 variables, 2249

continuous variables and 3041 constraints. To develop the trade-off curve the ϵ -constraint method was used. DICOPT required 3.5 minutes while BARON required about 100 hours. The solution involving shortest lead time of 8.85 days had an NPV of \$158 million, while the longest lead time was 14.42 days at a much higher NPV of \$1,261 million.

Fengqui is currently addressing the simpler planning problem in which the structure of the supply chain is given, and where major decision variables are the safety stocks. In order to address this problem he is exploring the incorporation of inventories for measuring lead times using stochastic models from inventory control theory.

Scheduling of Batch Multiproduct Plants

New Development: **Publication of review paper**

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

At Carnegie Mellon, Pedro first examined the single stage problem with parallel lines. Pedro found if that he does not use a common time grid for the parallel stages, but that rather uses a multiple time grids for each stage, then the RTN MILP model can be solved almost as fast as the hybrid MILP/Constraint Programming model. He solved problems ranging from 12 orders and 3 units, up to 30 orders and 5 units for the cost minimization case. Another interesting result that emerged was that Pedro solved the discrete time model with up to about 400 time intervals in order to obtain exact or very close approximations. The surprising point here was that while the discrete time model was slower for the smaller problems, it did not experience an exponential increase in time. In fact the times ranged from 2.5 to 27 seconds for all the test problems. When the objective is minimization of earliness the discrete time model performed the best followed by constraint programming. This comes to show the importance of objective functions in scheduling problems.

In the next phase, Pedro investigated the optimal scheduling of multistage plants. In this case he performed a non-trivial extension of the multi-time grid RTN MILP model for a single stage. He also examined in detailed a sequential MILP model that had been proposed previously by Harjunkoski and Grossmann. He performed extensive numerical experiments using as objective functions cost minimization, minimization of makespan, and earliness minimization. The problems ranged from 6 orders, 4 units, 2 stages to 10 orders, 8 units, 4 stages. His results showed that constrained programming tended to be the more effective solution method for makespan minimization. The sequential model proved to be best for earliness minimization, while the proposed model performed best for the cost minimization criterion. On an overall basis, the discrete RTN model was also competitive. Here again the discrete-time formulation was shown to have very good performance, particularly for total earliness minimization, despite generating very large MILPs when considering the exact problem data. The main conclusion was that for the multistage case not a single model proved to be the dominant one. This work also led to a manuscript that has been published.

The extension to handling changeovers in multistage plants Pedro has completed recently by developing two new continuous-time formulations for the short-term scheduling of single/multistage plants. The formulations rely on the use of multiple time grids, one per equipment resource. While one formulation uses binary variables linked to such tasks, giving rise to 4-index binary variables, the other maintains the 3-index binary variables of the previous model and changes one set of constraints to make it possible to handle sequence dependent changeovers. Both formulations were shown to be very efficient in single stage problems with the most surprising result coming from the fact that the 4-index binaries formulation was found to be slightly better than its 3-index binaries counterpart, despite featuring a number of binary variables that can be up to one order of magnitude larger. As the number of stages increases, the performance of the multiple time grid formulations decrease steadily and feasibility may even be compromised. The other goal was to provide a critical review of other approaches that are suitable for this specific type of scheduling problem. These included an RTN-based discrete-time formulation, a continuous-time model with global precedence sequencing variables, a constraint programming model and a hybrid MILP/CP model. A total of 39 examples were solved and the results, together with those of the two previous works, allowed Pedro to identify the main features, strengths and weaknesses of each approach, which were summarized in a comprehensive table. Overall the best model proved to be the continuous-time formulation with global precedence sequencing variables. The paper describing this work is listed as a reprint.

Pedro is currently exploring an RTN model for a simplified version of the Dow problem that Muge is addressing (single stage reactors).

Simultaneous Scheduling and Control

New development: **Simultaneous MINLP model for cyclic scheduling of multiproduct CSTR reactor**

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

This is a collaboration with Antonio Flores from the Universidad Iberoamericana (Ignacio's alma mater). Antonio, being a control person, has been motivated by the idea of using dynamic models for control in scheduling problems. Given our interest in the area of scheduling, we decided to join forces in a work in which the basic idea is to combine a scheduling optimization model, with a dynamic model for the optimization and control of the transitions. In this work we have addressed the simultaneous scheduling and control problems for a continuous stirred tank reactor (CSTR) that produces multiple products within a cyclic schedule that involves sequence dependent transitions. In the previous newsletter we reported a formulation where integer variables are used to determine the production sequence and continuous variables take into account production times, cycle time and inventories. The scheduling part of the model is similar to our previous work with Jose Pinto. Because, dynamic profiles of both manipulated and controlled variables are also decision variables, the dynamic part of the model is formulated with DAEs. The resulting problem can then be cast as a Mixed-Integer Dynamic Optimization (MIDO) problem in which the objective function includes income from sales of products, inventory costs and transition costs that takes into account through quadratic deviation terms, the amount of off-specification material produced during product transition. To solve the MIDO problem the MIDO problem is transformed into an MINLP using orthogonal collocation, where initial guesses on the duration of the transitions must be provided. These are then revised in a subsequent optimization.

Antonio and his student Sebastian Terrazas-Moreno have developed a new MINLP formulation to simultaneously solve the scheduling and control problems in polymerization reactors during a cyclic manufacturing operation. In contrast to the previous model, the problem need not be solved sequentially by iteratively assuming fixed lengths for the duration of the transitions. Another interesting feature of the model is that by assuming that the performance of each polymer is only dependent of the initial conditions, the problem can be formulated in terms of 0-1 variables for assigning products to slots. The transitions are then simply computed from the difference in the initial conditions. This leads to a much smaller number of 0-1 variables compared to the case when sequence dependent transitions are explicitly modeled. Two case studies related to the polymerization industry were solved: the isothermal free radical bulk polymerization of styrene, and methyl-methacrylate polymerization. In the latter the production of four grades (A,B,C,D) was considered corresponding to molecular weight distributions of 15000, 25000, 35000 and 45000, together with complex kinetic models. The predicted cycle time was 172,2 hrs with an optimal sequence of D → A → B → C in which the dynamics of the transitions were explicitly accounted. The required CPU with DICOPT for the corresponding MIDO problem using orthogonal collocation was 70 secs. The paper describing this work is in the section of references.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: **Rosanna Franco (started July 2006)**

Rosanna Franco has joined our group as a research assistant. As a first step she has updated some of the web-interfaces that Gabriela Garcia has developed and that are available in:

<http://newton.cheme.cmu.edu/interfaces>

She has also started to develop a new interface for integrated water systems, based on the work of Ramkumar Karuppiah This interface should be available in the next few months..

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

Synthesis:

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

Batch design:

BATCHSPC	MINLP and MILP models for multiproduct batch plants single product campaigns (Kocis, Voudouris)
BATCHMPC	MILP model for multiproduct batch plants mixed-product campaigns (Birewar, Voudouris)

Scheduling:

STN	State-Task-Network MILP formulation for scheduling multipurpose batch plants. Both the the Kondili, Pantelides and Sargent (1993) model and the Maravelias and Grossmann (2003) are implemented.
PARALLEL	MINLP continuous multiproduct scheduling on parallel lines Features feasibility preanalysis (Sahinidis)
MULTISTAGE	MINLP continuous multiproduct in multistage plants (Pinto)
CYCLE	LP/MILP aggregate flowshop scheduling (cycle time/makespan) Includes loop tracing algorithm (Birewar)
STBS	MILP short term multistage scheduling (Pinto, Bolio)
CRUDEOIL	MILP model for refinery scheduling (Lee, Pinto)
DECAY	MINLP model for scheduling of clean-up of parallel furnaces (Jain)
UTILPLAN	MILP multiperiod model for utility plants (Iyer)
PRODEV	MILP model for scheduling of tests in new product development (Schmidt, Najimas) MILP for resource scheduling in new product development (Jain, Maravelias)

Planning:

PLANNER	MILP multiperiod model for capacity expansion in process networks (conventional and lot sizing model) (Sahinidis, Norton)
MULTISITE	MILP model for planning the selection of processes and capacity expansion in different geographical location and accounting for transportation costs (Turkay)
GREENPLAN	Bi-criterion MILP model for selection of processes that maximize the net present value and minimize toxicity (Drabbant)
NETCHAIN	Multiperiod MILP for supply chain optimization of multisite facilities with flexible processes, intermittent deliveries, changeovers and inventories (Bok/Iyer)

Steinar Hauan's Group

Agent Systems in Engineering Design and Optimization

**Students: John Siirola (PhD, completed May 2005), and Israel Owusu
(PhD, started Jan 2004).**

BACKGROUND

The main idea behind agent systems is to enable the study of
large-scale engineering and design problems where:

- the models are complex, highly nonlinear and definitely non-convex
- many of the calculations fail routinely
- the problem has many local optimum
- the solution space of discrete alternatives is enormous

The underlying approach asserts that our computing capabilities will increase significantly over the next decade and that the computational resources will be available in the form of distributed computer clusters. We believe this will change our perception of "effective computing strategies": instead of creating algorithms that reach a result in the minimum number of algorithmic steps, it will become more important to be able to use the available -- but distributed -- computing resources in an efficient manner. This represents a shift in thinking from CPU time to wall clock time.

A key feature in our approach is the use of an agent-based architecture. In these systems many computational agents -- or individually executing algorithms -- attack different or even the same parts of the problem. There are also agents that remove bad solutions. All these agents share total and partial solutions as they progress. This sharing is very low bandwidth relative to the information developed by any agent internally. Experience shows there is considerable synergy among these agents, often reducing the time to find solutions by surprising amounts. For example, an agent may discover another agent has produced a particularly good new point from which it thinks it can make rapid progress. Or it may find a solution that gives it a much improved bound over any it has found by itself. These systems are like creating an army of ants to attack the problem, in the hopes that one of them will reach a desired solution. Parallelism comes by having the agents operate more or less autonomously and in parallel on several computers. But if computing is fast and cheap - why not?

With the completion of John Siirola's thesis, the fundamental implementation of the agent system and its control structure has been established. We have completed preliminary studies of multiobjective optimization for NLP, MIP and (simple) MINLP systems and demonstrated the conditions under which the agent system performs well compared to traditional approaches. We have also established the concept of "Polymorphic Optimization" wherein the agent system simultaneously consider more than one mathematical model of our physical system that each (de)emphasizes a particular aspect of the model.

PROGRESS

Israel has spent the last semester implementing his method for distributed optimization of supply chains. Some sample results are starting to appear; the solution times are (much) better while the solution qualities are similar to traditional approaches.

Microscale Chemical Synthesis and Sensing

Microsystems is an extreme case of process intensification with general advantages compared to conventionally sized equipment as follows:

- improved conversion and selectivity in chemical reactions due to potentially better control of local mixing and heat transfer as well as a surface to volume ratio,
- capacity scaleup by device replication and not change of size avoids normal redesign issues when moving from laboratory equipment to pilot plants to production facilities,
- improved safety as the small amount of materials and energy present significantly reduces the potential impact of accidents and spill,
- clean and cost-effective production of small volumes through the use of cheap, one-time production equipment with no need for downtime and batch cleanup or risk of contamination, and
- reduced requirements for physical space and power.

Applications are emerging in the areas of sensor systems, microscale chemical synthesis, high throughput screening, environmental monitoring and medical sciences. The goal of this research is to adapt and expand current algorithms for process design into this new domain. At present, two directions are being actively pursued: (1) microscale fluid flow and chemical reactions, and (2) gravimetric sensing of biological molecules

The overall goal in microscale process design is to find the proper level of modeling detail to capture fluid flow, chemical reactions and heat transfer to address system level issues such as flow configuration, unit layout and operational procedures. With the proper experimental building blocks, we aim at treating these systems as multi-purpose and multi-period batch plants with special methods for dealing with surface-, heat- and end-of-pipe as well as coordination of clustered arrays for high throughput testing and production. There are 3 key issues in this project: (a) identification and modeling of relevant microscale effects, (b) how to generate reduced order models suitable and computationally feasible in a multi-unit optimization framework, and (c) shape- and parameter optimization of the resulting microscale unit operations. One of the key aspects is to understand the underlying physics and capture the behavior in a sufficiently simple model; this is being pursued with collaborators in ECE and ME.

Specific Projects:

(a) Microscale Total Analysis Systems

Students: Anton Pfeiffer (PhD, graduated Apr 2006) and Xiang He (Ph.D., started Jun 2003)

Collaborators: Tamal Mukherjee (ECE), Jim Hoburg (ECE) and Qiao Lin (ME)

BACKGROUND

Microfabrication processes have enabled manufacture of micro-sized channels, pumps, valves, mixer components and reactors. Integration of these components have enabled the creation of on-chip systems that span sample collection, preparation and analysis of biological materials, drug screening and chemical synthesis. Existing lab-on-a-chip systems tends to consist of relatively few components as the development of each such microscale unit operation continues to require empirical optimization and trial-and-error approaches. Long and expensive development cycles are acceptable for high-volume products where the equipment and process life times are measured in years and a few percent performance improvement translates to large profit. However, the wide variety of biological applications such as genomics, proteomics, therapeutics, diagnostics and a wide-array sensor systems implies the need for many customized designs instead of a few high volume products. Our work aims to create computer tools to aid in the development of two types of customized microfluidic devices: (a) integrated system wherein multiple microfluidic components are combined to form a complete single-function analysis system, and, (b) multiplexing systems where independent subsystems are combined physically on the same structure to provide parallel and/or redundant measurements.

The core idea of this work is to reduce the design and verification time for custom-designs from months and years to days and hours by use of component models and software tools for simultaneous performance optimization, layout and routing of the individual chips in question.

PROGRESS

Xiang has completed the analysis of geometry in LoC serpentine channels and is currently writing the paper. It turns out that many published experimental designs for electrophoretic separation on a microchip are unnecessary complex and could be replaced by smaller, simpler and often standard designs.

(b) A MEMS-based Gravimetric Biosensor

Students: Michael Bartkovsky (Ph.D., graduated Aug 2006), Jane Valentine (Ph.D., started Jan 2003),

Collaborators: Todd Pryzbycien (Biomedical Engineering) and Gary Fedder (ECE).

BACKGROUND

This work aims at creating a MEMS-based device capable of detecting picograms of biological target molecules. The basic principle is to cause a shift in resonance frequency for a polymer membrane by specific chemical functionalization of its surface. The membrane has characteristic dimensions in the millimeter range and prototypes have been used in microphones and speakers by our ECE collaborators.

There are four major tasks in this project:

- (a) fabrication of a CMOS/polymer membrane with integrated capabilities for actuation and capacitive sensing.
- (b) chemically specific functionalization of the membrane surface such that target molecules get adsorbed with the highest possible selectivity
- (c) creating a clamshell packaging in which liquid samples may be brought in contact with the membrane surface.
- (d) computer aided optimization of system parameters – including device geometry, functionalization density and scanning frequencies -- for single membranes as well as arrays of such.

PROGRESS

Mike completed his thesis and demonstrated the ability to detect femtogram of proteins using our sensor. This is significantly more sensitive than we have seen in other published sensing approaches.

Jane has tested and implemented several strategies for sensor array optimization. The most promising one so far separates the problem into first solving a problem in the frequency domain before converting it to a constrained placement problem on the actual surface of the membrane. The concern and current investigations aims at determining whether optimality can be achieved this way or if a simultaneous solutions is required.

Design of Multiproduct Reactive Separation Plans

Students: Scott Turnberg (Ph.D., started Jan 2005)

BACKGROUND:

Reactive distillation is a multifunctional process combining product conversion and separation inside a single piece of equipment. While the process has been demonstrated to significantly reduce both the capital and energy cost for highly non-ideal physiochemical systems, systematic design methods for generating and comparing design alternatives have been slow to evolve.

This projects seeks to combine recent analytical and algorithmic advances in the theory of reactive separation systems with the design of multiproduct plants for flexible production of acetate and oxygenate series. The main deliverables of the project will be:

- (a) an algorithm capable of rigorously determining whether a particular set of reaction and separation tasks may feasibly take place in a single piece of equipment,

- (b) a multi-objective optimization approach to assessing the economic trade-offs between the design alternatives generated,
- (c) extensive case studies on current sequential and integrated processes to identify the first generation of pilot plant experiments for multiproduct equipment.

It is a goal to carry out the systematic search for solutions in part (c) using the agent system.

PROGRESS

Scott has converted the feasible region analysis into a system that automatically generates a set of linear constraints for optimization of reactive cascades. These constraints control the movement of the composition profiles based on bifurcation analysis for reactive pinch point curves and enables automatic initialization of series of reactive separation case studies.

Erik Ydstie's Group

Modeling and Control of Distributed Process Networks

Student: Kendell Jillson (Ph.D.)

Kendell Jillson has developed very efficient methods for how to model and integrate very complex process networks in a stable manner. He has developed methods that show how such systems can be designed to be self-stabilizing and self-optimizing. He has also investigated the stability and control of supply chain network systems, and is also now beginning work on a project in collaboration with WVU and DOE-NETL on the modeling and control of an integrated gasification combined-cycle (IGCC) power plant. Also, Kendell will soon begin writing his PhD thesis, anticipating completion and defense in late March/early April.

We have 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. With visiting Professor Jie Bao (University of New South Wales, Australia), he has investigated and developed the stability and passivity theory further, and they produced a conference paper, "Passivity based control of process networks", submitted for the upcoming DYCOPS conference.

We have also developed a theory for plant-wide control and stabilization of complex process systems. We have developed structural conditions for stability and simulated a recycle-flowsheet with a reactor and distillation column. The paper describing these results has been submitted for review in the Int. Journal of Process Control.

Furthermore, we have looked at supply chain systems with networked behavior. Using Simulink, example systems were modeled and controlled to maintain inventory set points in each node or unit along the chain. Also, a pricing policy was introduced at each node, so that in a decentralized manner, nodes could both maintain their desired inventory set point and buy goods from the cheapest upstream sources.

Finally, in collaboration with Dr. Richard Turton from West Virginia University and Dr. Stephen Zitney (DOE-NETL), Kendell is beginning work on a project dealing with the modeling and control of an integrated gasification combined-cycle (IGCC) power plant.

Modeling and Control of Particulate Processes

Student: Christy M. White (Ph.D.)

Christy has worked with Erik on two different papers. The first addresses stability of nonlinear control through feedback linearization and will be submitted to the IFAC Symposium on Nonlinear Control. The second shows results of collaboration with consultants working for REC Silicon and will be submitted to a CVD journal. She will complete research as she compiles her thesis this semester.

The 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.

This 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. These results were presented at the AIChE meeting in Cincinnati. 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. Some results from this research will be presented at the Particle Technology Conference in Florida in May. The model and control scheme is being used for scale-up and control system design for production system under current development at SGS. It is expected 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.

Supervised Adaptive Control

Eduardo J. Dozal-Mejorada (Ph.D.)

Eduardo (Wayo) has been developing a new adaptive control method based on supervision. The method works by updating the control estimates only when new relevant information is obtained. The technique is based on a dual-model approach. The main objective of this research is to develop methods for optimal control of fully (or partially) unknown systems which do not rely on full state feedback. Simulation studies have been used to illustrate the set point tracking capabilities of the algorithm. Experimental studies on a heat exchanger have shown that the algorithm successfully suppresses output bursting.

The main objective of the work is to improve robustness of adaptive process control. The proposed method is related to the deadzone idea since it relies on the idea of turning estimation off once a given criterion has been satisfied. Adaptive prediction theory can be used to show that the prediction error of the second model converges to an optimal estimate of the plant disturbances. This in return can be used to show that the parameter estimates and controller converge close to optimal performance. Currently, theoretical results are being developed. The primary objective is to show that the dual model supervised adaptive control algorithm is robust with respect to small model/plant mismatch and bounded disturbances.

Furthermore, the use of input output data allows us to focus modeling attention on the low order (observable and controllable) dynamics while the fast (poorly observable) dynamics are allowed to drift and it is therefore suitable for optimal control with wide separation of time constants. It is our belief that the technique should be very well

suited for multi-variable process identification using real time process data. In this spirit, a proposal has been submitted to Shell Global Solutions' Westhollow Technology Center to work closely together with the technique in order to test the applicability of the algorithm to real MIMO process data.

The advantages of this adaptive algorithm over other traditional optimization approaches include: 1) it uses current process models, 2) it can handle multiple objective functions, 3) it only applies a subset of all process states, 4) it self-learning, and, 5) it is appropriate for steady-state or dynamic models. We have developed theoretical convergence and stability results for the exact-matching case and have started working on the robustness problem. Successful implementation has been applied to two case studies: 1) optimization of biomass production in a bioreactor, and, 2) optimization of silicon production in a reactor. These results were presented at the AIChE meeting in Cincinnati.

Wayo and Kendell have developed a method for optimization of complex supply chains using Kendell's network theory. They show that by focusing on value added and cost minimization in a distributed supply chain it is possible to achieve global optimality without a central coordinator if the activity rates are positive,

Passivity Based Control and Real Time Optimization of Multi-Phase Reactor Systems

Student: Yuan Xu (Ph.D.)

Yuan Xu is working on stability analysis and batch reactor operation. In the stability side, he is extending the analysis tool from thermodynamic to more complicated problems. In the batch operation side, he is developing an adaptive control method for batch problems with uncertainties. His application domain is the carbothermic reduction of aluminum oxide to form aluminum.

The focus of this research is on passivity-based control of multiphase systems with reaction transport (diffusion and convection). To study this type of system, a metallurgic process has been chosen involving the carbothermic reduction of aluminum. This process 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. Proportional control is currently being used to explore the controllability, stability, and sensitivity of the system. Future work will be directed toward interfacing the FACT thermodynamics program with MATLAB via a MEX Interface. This will allow for the model to handle ranges of temperatures and compositions without extra work needed to determine equilibrium constants, activity coefficients, and extent of reactions. Another future improvement will be to incorporate computational blocks using the SIMULINK tools in MATLAB. 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.

Thermodynamics and Process Networks

Students: Luis Antelo (Ph.D. Univ of Vigo, Spain)

The aim of this research is to develop new foundations for control and optimization of large integrated, networks of chemical processes. We use the formalism of irreversible thermodynamics and the passivity theory of nonlinear control as a basis for this theory. However, there are severe limitations that need to be overcome when we extend these methods to problems that include coupled fluid flow, heat and mass transfer.

Luis has continued Felipe's work on the flash systems stability and he is currently studying how he can extend these to distillation by combining his ideas on using the Gibbs-Duhem equation with the algebraic methods of Chad Farschman and the Lagrangian/Eulerian decomposition of Duncan Coffey. He has also developed a new theoretical framework for plantwide process control which we are currently testing in simulations. Luis went back to Spain in the beginning of December. He will come back to visit us for three months next fall.

Modeling the Vapor Recovery Reactor in Carbothermic Aluminum Production using Multi-Scale Modeling Methods

Student: Mohit Aggarwal (co-supervised with Prof. Lee White) (Ph.D.)

Mohit just joined the group in November. He will start out his PhD by developing a model for the vapor recovery section of the carbothermic aluminum process under development by ALCOA. In this process aluminum is produced in a high temperature (2000C) two stage process. A significant amount of aluminum vaporizes from the aluminum reactor and this aluminum must be recovered in a vapor recovery column in order to maximize the production yield and save energy. We will model 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. This work is a continuation of Vianey's modeling work (PhD/PostDoc 2004). Mohit will develop a three phase (liquid/solid/gas) multi-scale, simulation model which will be used for system design, scale-up, economic evaluation and control studies.

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