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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GENERAL NEWS

CAPD e-News. We sent on April 27 our first e-newsletter. We decided that we will issue a total of four newsletters per year. Two will be the extensive report on projects with preprints as we have done in the past, the two others will be brief e-Newsletters that will contain short announcements as well as information that we think will be useful to the CAPD members. We plan to issue the e-Newsletter in April/May and October, while the extensive report will be issued in August and December. Please let us know your reaction to the e-Newsletter and to the new arrangement.

Erik Ydstie developed a new short course on Advanced Process Control. The course covers control system structure in multivariable systems, system identification, predictive control, real time optimization and process data analysis. The case studies include moving bed reactor control, glass furnace, stirred tank reactors, fluid flow control and plantwide control and optimization. The first set of lectures were presented for the Emerson control group. Erik also started a **new company** called iLS (Industrial Learning Systems). The company will seek to industrialize adaptive and learning control methods. Development partnerships have been initiated with Dow, Alcoa, Emerson and Integ. The aim is to beta-test a single loop adaptive predictive controller early next year and a multivariable controller in 2007. The company is co-owned by CMU, Rajeev Kutty and Michael Helman (former Tepper students) and Erik.

Congratulations to our Ph.D. students who had their Ph.D. exams and graduated in May. **Vikas Goel,** student of Ignacio, has joined the Upstream Research Center of ExxonMobil in Houston. Vanesa de la Torre, student of Larry, has completed her Ph.D. this year. **Maame Poku**, student of Larry, has joined BP Chemicals in Naperville. **John Siirola**, student of Art and Steinar, is currently postdoctoral fellow in the department. **Cong Xu**, student of Larry, is currently a postdoctoral fellow in the department. Congratulations to **Yoshi Kawajiri**, who passed his proposal exam this summer.

Several of our students are in internship positions this summer: **Muge Erdirik** at Dow Chemical, **Ramkumar Karuppiah** at ExxonMobil, and **Carl Laird** at IBM. **Christy White** spent three months in Belgium at Universite Louvin la Neuve where she visited Dr Denis Dochain. She worked on the problem of developing state and parameter estimation methods for particulate processes. The visit was funded by the National Science Foundation. **Eduardo Dozal** spent three months at the Shell development center in TX as an industrial intern working on supply chain related problems.

Jose Caballero from the University of Alicante visited Carnegie Mellon in July collaborating with Ignacio in the area of synthesis of thermally coupled distillation columns. **Metin Turkay** from Koc University and **Bulent Karasozen** from Middle Eastern Technical University have visited in July and are collaborating with Larry in the area of hybrid systems. **Fernando Mele,** Ph.D. student from Polytechnic University of Barcelona (Puigjaner's group) visited Ignacio's group for 5 weeks to do research in the area of supply chain optimization. **Sergio Frausto**, Ph.D. student of Vicente Rico at the Instituto Tecnologico de Celaya in Mexico, is visiting Ignacio's group for 6 months working in the area of stochastic optimization for planning of process networks. **Carlos Mendez,** who was a postdoctoral fellow in Ignacio's group for almost two years, has moved to the Polytechnic University of Barcelona, where he is working in the group of Professor Luis Puigjaner. Carlos, however, continues to collaborate in projects with ABB and BP. **Pedro Castro** from INETI (Instituto Nacional de Engenharia, Tecnologia e Inovação), Lisbon, Portugal, who worked in Ignacio's group for almost one year in the area of batch scheduling, has returned to Portugal. **Minhwan Park** from KAIST, Korea, has also returned to his country after a 6 month visit working in Ignacio's group in the area of contract modeling.

ENTERPRISE-WIDE OPTIMIZATION INTEREST GROUP

The new special interest group on Enterprise-wide Optimization has been created as part of the project **"Computational Models and Algorithms for Enterprise-wide Optimization of Process Industries"** that has been funded by the Pennsylvania Infrastructure Technology Alliance (July 1, 2005-June 30, 2006). The goal of the project is to provide a comprehensive set of computational capabilities for addressing the integrated planning, scheduling, real-time optimization and inventory control of process systems. 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 total funding for year 1 is $518,194 (July 1, 2005 to June 30, 2006). PITA will provide $205,301, and we are leveraging $250,343 from Federal and University grants. The remaining $62,500 will come

from five companies, under the special rate of $12,500 for members of the CAPD. The companies who have agreed to participate are ABB, Air Products, BP America, Dow Chemical, and ExxonMobil. These companies have supplied case studies that will be undertaken by the EWO faculty and students. There will be two meeting of this group on **October 3, 2005**, and on **March 15, 2006**, to review the progress of the work.

2006 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on **March 13-14, 2006**. 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. There will also be a dinner that evening at Le Mont Restaurant. The second day is devoted to final year student presentations. Last year the feedback we received was very positive. If you have any additional thoughts or suggestions, please let us know.

2006 CAPD SHORT COURSE

Our short course, ***Process Modeling and Optimization for Process Engineering*** will be offered on **May 31- June 6**, **2006**. In the past we were very pleased with the outcome of this course, as we have had attendees from around the world, both from industry and academia. For this year, the course has been extensively revised and includes the following modules:

a) Conceptual Design - taught on Wednesday and Thursday (May 31-June 1), with focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.

b) Optimization - taught on Friday and Saturday (June 2-3), 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 5-6), 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.

The course included extensive workshops where participants obtained hands-on experience with various software packages. Course materials included extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in attending this course next summer, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

PANAMERICAN ADVANCED STUDIES INSTITUTE ON PROCESS SYSTEMS ENGINEERING

Ignacio Grossmann is organizing together with **Jaime Cerda** from INTEC, Argentina, and **Jose Pinto,** from Polytechnic University and University of Sao Paulo, the PanAmerican Advanced Studies Institute on Process Systems Engineering (http://cepac.cheme.cmu.edu/pasi.html) that will take place in Iguazu Falls, Argentina, August 16-25, 2005. This is a workshop that is aimed at advanced graduate students. The major areas that will be covered are Optimization, Product and Process Design, Supply Chain Optimization and Process Control. About 50 graduate students will participate (50% from US), as well as several professors and researchers from Petrobras. The course material, slides of presentations, papers for background reading and GAMS and Matlab input files are now available 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.

CAPD REPORT SERIES

Along with our web sites we have initiated a technical report series that covers the research output of our center. In addition to the reports that are regularly sent to our members, we are cataloging these reports on the web sites mentioned above. This allows us and other researchers to refer to these reports prior to their publication.

EXECUTIVE SUMMARY

Larry Biegler's Group

The past few months have seen a number of applications of dynamic optimization problems in the following areas:

Some time ago, we proved an equivalence of the optimality conditions for optimal control and our simultaneous nonlinear programming formulation based on orthogonal collocation on finite elements. **Shiva Kameswaran** has recently shown some very useful extensions to this work. He has shown an extension of the equivalence to Radau collocation, both for unconstrained and endpoint constrained problems. Two papers that describe these concepts are listed below.

Nonlinear Model Predictive Control strategies are being explored with dynamic optimization tools centered on IPOPT. **Juan Arrieta** has developed NMPC strategies to determine near optimal trajectories for conflict resolution in low-thrust satellites. This is described in a publication listed below **Carl Laird** has expanded the source detection approach for municipal water networks in detecting contaminants in water network nodes. Publications that describe this work are listed below. Finally, **Victor Zavala** has started a new project on NMPC for large-scale polymerization processes.

For periodic adsorption applications**, Daeho Ko** and **Seth Knaebel** have extended the optimization formulation of Dr. Ling Jiang (now at Air Products) to the gPROMS modeling environment. As noted in a reprint below, both have done optimization on small pressure swing adsorption (PSA) cycles with binary separations. The optimization strategy appears to be fast and reliable and the resulting solutions show significant performance improvements over existing processes. In addition to this work, **Yoshi Kawajiri** is currently exploring similar optimization strategies for Simulated Moving Bed applications, the liquid-solid analog of PSA. A publocation that describes this work is listed below.

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 Waechter**, 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.html.

This summer, **Carl Laird** and **Andreas Waechter** have migrated the FORTRAN code for IPOPT into an object-oriented code written in C++. The resulting package leads to a much cleaner interface to modeling environments as

well as a more efficient implementation of the algorithm. Finally, the object-oriented code allows for greater flexibility 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.
- **ROMeo** – Recently, **David Ternet** of Simulation Sciences developed an interface between IPOPT and ROMeo, a widely used process modeling and optimization tool for real-time applications. IPOPT is currently being tested and compared with the current OPERA package by **Maame Poku** on a number of large-scale process problems. While ROMeo provides only provides exact first derivatives, it works well with the limited memory BFGS option in IPOPT.

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 can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package, as well as IPOPT will be enhanced further by the development of a number of interfaces to optimization modeling platforms including CAPE-OPEN. A paper that describes this work is listed below.

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

In the area of optimization **Nick Sawaya** has continued working in the development of cutting planes for nonlinear disjunctive problems, has completed a short note on the handling of the nonlinear constraints for the convex hull reformulation, and has developed a number of new test problems for the CMU-IBM MINLP open source code project. **Lorena Bergamini's** manuscript has been accepted on the new method for the global optimization for the logic-based OA method that relies in the use of piecewise linear underestimators. **Aldo Vecchietti**, has continued to expand the capabilities in LOGMIP, a GAMS-based code for disjunctive programming (http://www.ceride.gov.ar/logmip/). **Ashish Agrawal** has applied concepts of Type Theory for the reformulation of disjunctive programs and has produced software written in ML to do the automatic reformulation.

In the area of process synthesis **Ramkumar Karuppiah** completed a manuscript on the synthesis of integrated process water systems for which he has developed a new global optimization algorithm that combines spatial search with piecewise linearization. He has also started the extension to the case of global optimization under multiperio operation. In a joint collaboration project with BP, **Carlos Mendez** has performed the optimization of refrigeration systems in order to incorporate it in the superstructure optimization of a crystallization process for the separation of paraxylene. In a joint collaboration project with **Mike Domach, Soumitra Ghosh** has been applied concepts of the Analytical Hierarchy Process by Setty for screening of NMR analytes for determination of metabolic flux maps. **Jose Caballero** in Alicante has developed a new superstructure for thermally coupled distillation columns and used symbolic logic for generating all the feasible configurations.

Vikas Goel completed his PhD including the implementation in C++ of a Lagrangean based branch and bound method for solving multistage stochastic programs in which the scenario trees are dependent of the design decision. He is applying this technique to the planning of gas fields. **Bora Tarhan**, a new PhD student, has started to address the problem of optimal planning of process networks with uncertain yields qand in which time varying uncertainties are considered as well as possibility of installing pilot plants for reducing uncertainty. **Sergio Frausto**, a new visitor from Mexico, is working on a two-stage programming model for strategic supply chain with uncertain demands that are described by continuous distributions. The last manuscript of **Christos Marvelias** that derives the STN discrete time model; as a special case of the STN continuous time model has been accepted for publication. **Muge Erdirik** has completed a manuscript in the area of simultaneous planning and scheduling for continuous multiproduct plants in which she has developed a decomposition scheme that makes use of an aggregated MILP model combined with logic and capacity cuts. **Carlos Mendez** has completed a very comprehensive manuscript that provides a review of the area of short-term batch scheduling. **Pedro Castro** has been investigating various formulations for multistage problems with parallel units, including a novel RTN MILP formulation. Also, in conjunction with Carlos Mendez and ABB (Iiro Harjunkoski and Marco Fahl) he has developed a sequential decomposition strategy for complex multistage batch plants. Finally, **Minhwan Park** developed cost models that reflect different contracts for supply chain optimization problems for which he has used a disjunctive programming approach.

Steinar Hauan's Group

John Siirola (co-advised by Art Westerberg) has completed his PhD work on design and implementation of an agent system for distributed optimization. His last contribution was to demonstrate how the agent system may be used to improve upon the solution times for MIP problem by sharing intermediate solutions and good bounds within the Branch & Bound framework.

Anton Pfeiffer has demonstrated the simultaneous design, layout and i/o routing for multiplexed electrokinetic separation systems on a microchip; the paper describing the model and approach is currently in press for a special issue on design automation tools for IEEE. The next -- and probably final -- step in his graduate work is focused toward implementing a system simulator and subsequent algorithms for the automatic design of multi-unit Lab-on-a-Chip system which combines arbitrarily connected units with mixing, reaction, separation, injection and detection.

Xiang He -- working to create a reduced order model for chemical reactions in microsystems -- has implemented and tested a modeling approach for fast and accurate solution of the convective reaction problem based on the Method of Lines. Combined with her previous models based on a discretized network of PFRs, the models are expected to cover all situations to be encountered in the multi-unit LoC design framework developed by Anton.

Mike Bartkovsky (experimental focus) and Jane Valentine (modeling focus) continue their work on MEMS-based biosensors. Mike has designed and fabricated a 4th generation membrane chip with fully integrated circuits for actuation and detection. As of July 2005, all the mechanical and electronic components on the chip have been characterized and verified to operate as expected; the next step is to coat the physical structures with a polymer and perform chemical binding experiments in liquid. Jane has completed her work on a reduced order (analytic) model for predicting the frequency shifts resulting from partial chemical functionalization of the membrane. Her analysis has demonstrated how proper localization of binding regions may improve the sensitivity by a factor of more than twenty and also provides the path for array design. Papers are in their final stages of preparation for both the experimental and mathematical work on these sensors.

Murni Amhad is designing flowsheets for protein separation by liquid-liquid extraction in the presence of multiple contaminants. Over the last months, she has completed her framework for multi-unit systems with both forward and backward extraction of target proteins. The next step is to devise an algorithm wherein the global recycle streams are combined with fresh feed of polymers and salts in a way where the composition of all extractive units remain in the two-phase region for any set of inputs.

Israel Owusu -- working on asynchroneous approaches to distributed Enterprise Resources Planning -- has implemented a set of models that emulates the planning and scheduling of a set of multiproduct batch plants. The key feature of this model is that we may explicitly control the information exchange of demands, capacity and partial schedules that is passed between each plant in the overall set. This allows us to quantify the effects of

information sharing and subsequent impact on global efficiency under different demand scenarios and time horizons for production planning and fulfillment schedules.

Scott Turnberg has started to work on the design of multi-product and multi-purpose reactive separation plants. As a first step, he has implemented Matlab MEX files for Auto2000 and used them to design feasible product composition regions for quarternary non-ideal systems.

The Beowulf computer cluster has again been expanded. In addition to server infrastructure upgrades, a grant from Intel Academic Relations was used to increase the capacity to more than 200 CPUs and 600 Gflops.

Congratulations

John Siirola completed his Ph.D. thesis while Jane Valentine passed her proposal exam.

Erik Ydstie's Group

The Ydstie research group works on developing advanced modeling and control system methods for chemical processes. The work is distributed along two distinct axes. The first axis concerns how to use process physics and passivity based control theory to develop distributed simulation and control methods for chemical process networks. We are especially interested in developing methods that integrate physics, computation and communication in coherent and stable ways. The second axis is based on the idea of incorporation learning and adaptivity in control and optimization. We are especially interested in studying how we can learn and adapt simple representations of optimal control (discrete and continuous decision making) in complex systems.

Christy White has developed an efficient way to represent and model particulate processes. She has developed inventory control approaches for such processes and a general approach for state and parameter estimation. The problem she is working on is motivated by the direct reduction Saline to form high purity silicon for the photo voltaics industry.

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 is currently adapting the modeling paradigm so that it can be used to represent bio-processes.

Eduardo Dozal has developed a new method for real time optimization which can be used to solve complex problems in non-convex optimization. The method works by filtering out "surface roughness" and embedding the high dimensional problems in a low dimensional input output representation of the system to be optimized.

Yuan Xu joined the research group in January. He is working on stability analysis, distributed simulation and batch chemical control. He uses passivity based methods and integrates it with non-equilibrium thermodynamics. His application domain is the carbothermic reduction of aluminum oxide to form aluminum.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: Carl Laird (Ph.D. started Fall, 2001)

As a result of several generations of Ph.D. students, we now have a general strategy for 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 Waechter. This code has become a core algorithm for many of the research projects described below. In particular, 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. The approach is described in the reprint below. 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 a publication below. Finally, Carl is spending the summer with Andreas Waechter at IBM to complete development on the next version of IPOPT. 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. Moeover, as noted above, the new code provides a much easier interface to modeling environments.

Barrier (Interior Point) Methods for Nonlinear Programming in Process Engineering

Researchers: **Maame Poku (Ph.D. completed Spring, 2005)**
Brian Baumrucker (Ph.D. started Fall, 2004)

This project considers an efficient strategy for solving nonlinear programs using interior point (IP) methods for process engineering. In particular, the IPOPT code is being widely used in Larry's group and elsewhere. Examples include both full space and reduced space versions for dynamic optimization, in OCC and DynoPC, respectively. In addition, the full space approach has been used in blending applications and in the solution of MPEC problems. **Maame Poku** has completed her PhD thesis and has taken a position with BP. She investigated the use of IPOPT for a number of process applications. In particular, she applied IPOPT with the AMPL interface to deal with nonlinear planning and blending problems. These problems have a large number of superbasic variables (degrees of freedom). As a result, reduced space NLP algorithms (like rSQP, MINOS, CONOPT and SNOPT) do not work well. Extensive results show that the full-space version of IPOPT works quite well on these problems. In addition, she applied this approach to data reconciliation and real-time optimization problems in SimSci's RomEO environment and has tested it on a number of large-scale real-time optimization problems. A publication is currently being prepared on this comparison. **Brian Baumrucker** has taken over this project 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.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: **Arvind Raghunathan (Ph.D. completed March, 2004)**
Prof. Ricardo Perez (Pontifical University of Chile)
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:

Arvind Raghunathan recently completed his Ph.D. and has accepted a position with United Technologies. 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.

Future work 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. **Brian Baumrucker** has recently joined the group and will be considering the developing of good MPEC formulations that model discrete decisions. 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

Students: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
Shivakumar Kameswaran (Ph. D. started Fall, 2001)
Victor Zavala (Ph.D. started Fall, 2004)

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

This 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 sabbatical visitor from the University of Iberoamericana, has demonstrated the advantages of this approach on a number of challenging polymerization processes. Moreover, he has recently extended this to consider the design of control systems for potentially unstable processes. A reprint that describes this approach is listed below. A number of research projects have 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 a collaboration with Prof. Marquardt's group at the Technical University at Aachen (RWTH). Here we have incorporated 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. In particular, Yi-dong has recently completed a polymer reactor study that was modeled in gProms and solved with DynoPC. This problem had over 300,000 variables and was solved in about an hour of CPU time. Further reformulations of this system, using a simple partitioning strategy,

have led to an optimization problem that is much better conditioned and can now be solved in only about 1000 CPU secs. A reprint that describes this approach is listed below. Finally, this approach can also be integrated into a two level optimization strategy that alternately solves the dynamic optimization problem for a fixed mesh, and then optimizes the mesh in an outer level; it easily allows for the addition of moving finite elements as well.

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. However, there are a number of limits to problem sizes that can be considered with this strategy. As a result, updates to IPOPT also need to be transferred to reduced space optimization strategies. We are currently adopting a MATLAB framework and coupled it with the AMPL modeling language. Domain specific prototypes have already been developed (as described below) 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 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. Two papers that discuss these properties in detail are listed below. Moreover, these results also point to the solution of singular control problems. These features lead to ill-conditioned KKT matrices, nonunique solutions and possible failure of the NLP solver. Based on the convergence analysis, we intend to develop reformulations that will regularize the KKT matrix and provide a consistent theory for more general optimal control problems.

Nonlinear Model Predictive Control Strategies

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.

Our current work extends these off-line strategies to on-line nonlinear model predictive control (NMPC). Here only partial solutions are considered for the aircraft trajectory and efficient NLP solutions are required in order to guarantee on-line performance and stability. Juan Arrieta has recently developed two prototype formulations: an NMPC strategy based on a detailed NLP solution and an MPC strategy based on solutions of QPs. Both of these strategies have demonstrated efficient partial solution strategies that allow conflict free flight in the face of many aircraft and obstacles. In particular he has shown that the NMPC strategy does no suffer from large deviations from the optimal trajectory in the nominal case; it has handled pop-up threats and incorporates limitations due to radar ranges. Juan 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. A paper that describes this approach is listed below.

Finally, the NMPC 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.

Large-Scale Optimization for Fuel Cell Models

Researchers: Cong Xu (Ph.D. completed Spring, 2005, joint with Prof. M. S. Jhon)

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. A reprint of this approach is listed below. Cong's current work deals with the optimization of hydrogen fuel cells and the incorporation of ancillary process models. 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.

Optimization and Control of Periodic Adsorption Processes
Student: Yoshi Kawajiri (Ph.D. started Fall, 2003)

Visiting Researchers: Vanesa de la Torre (PLAPIQUI)
Daeho Ko (Yonsei University)
V. Grant Fox (formerly Air Products)

In tandem with dynamic optimization projects, we are also developing more direct sequential strategies for the solution of dynamic optimization problems. These sequential approaches are easy to construct and have seen a lot of previous development in other research groups. An important (and time-consuming) aspect to these sequential strategies is obtaining sensitivities from the dynamic model efficiently. Fortunately, recent projects by Barton at MIT, Petzold at UC-Santa Barbara, and researchers at the Max Planck Institute have led to excellent software implementations that calculate sensitivities efficiently from large DAE process models. Also, these sequential approaches take advantage of 'off-the-shelf' solvers and do not require a heavy research investment as with simultaneous methods. As a result, we are embarking on large-scale dynamic optimization projects that combine our large-scale rSQP tools with efficient DAE solvers and sensitivity codes. One interesting benefit of this approach is that the most time-consuming elements can easily be parallelized with linear speedups.

To take advantage of these algorithms, we have completed a NSF/GOALI initiative with Air Products for the optimization of Pressure Swing Adsorption (PSA) systems. For this approach we have exploited existing models and implementations for the optimization of comprehensive, detailed PSA systems. Up to now, no satisfactory optimization strategies have been developed that can deal with these models. In her Ph.D. thesis, Ling Jiang has generated a number of interesting results for this project. She has been spending her summers at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, and automatic differentiation codes, like ADIFOR, to adsorption bed models created from the method of lines. In particular, she concentrated on developing detailed PSA bed models with hyperbolic and parabolic components that require special mass conserving discretization strategies to convert them to DAEs. Termed flux limiters, these discretizations allow the accurate tracking of steep fronts and discontinuities that frequently arise in PSA systems. Ling has successfully simulated and optimized cyclic steady state conditions for two PSA units, using Newton-type and tailored rSQP solvers. From this point she has demonstrated a framework that includes constrained simulation problems and design optimization problems on a number of PSA examples. *Results of her work show that this optimization strategy can reduced the power requirements for PSA systems by about 15% and the computational cost is an order of magnitude less that with conventional case study approaches* .More recently, she has implemented this approach to run in parallel on our Beowulf cluster; this leads to tremendous speedups in PSA optimization, as the sensitivity equations are trivial to

parallelize. Finally, this work has been applied to complex PSA systems for the separation of high purity hydrogen from refinery gases.

In addition, we are extending this PSA optimization strategy to a number of more complex systems, as follows.

- First, these systems are used for the sequestration of CO2 from flue gases. Previous work by Dr. Daeho Ko has shown that efficient optimization formulations can be developed in gProms. Dr. Ko is continuing this work with researchers at NETL in order to develop new sorbents for PSA and TSA operations for CO2 recovery.
- The gProms models have been extended to separations of H2 and CH4 by Seth Knaebel. He has modified these models with new isotherm data and also evaluated and optimized of a number of new PSA cycles. This work is described in a reprint listed below.
- Vanesa de la Torre recently completed her PhD thesis in Argentina. For her thesis, she has developed optimization models for PSA systems that address load following approaches induced by changes in product demand. These models will be used to develop MPC strategies for on-line control of a number of PSA processes. She has demonstrated this approach on a number of systems including air separation. A paper that describes this approach and application is listed below.

Finally, these successes have led us to consider applications in Simulated Moving Beds (SMB), the liquid analog to PSA. 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.

Yoshi Kawajiri recently completed his proposal exam and has been investigating efficient optimization strategies for these systems. Here optimization methods can be based on the single-discretization approach discretize the Partial Differential Equations (PDEs) only in the time domain and then integrate the resulting Differential Algebraic Equations (DAEs). 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 used the latter approach and has shown tremendous improvements in the productivity of SMB systems. Moreover, these were obtained almost two orders of magnitude faster than with sequential methods such as gProms. The approach also allows us to consider the design and control much more complex SMB systems. A paper that describes this approach is listed below.

Data Reconciliation for Steady State and Dynamic Processes

Researchers: **Nikhil Arora (Ph.D. started January, 1999)**
Shivakumar Kameswaran (Ph.D. started Fall, 2001)

Previously, Nikhil Arora (now with PraxAir in Tonawanda, NY) extended data reconciliation and parameter estimation strategies to both steady state and dynamic processes. Initially, he applied statistical tools to determine steady state conditions, classify measurements and observed model variables, detect data outliers and estimate model parameters. Nikhil has also developed specialized algorithms that deal more efficiently and reliably with these problem classes. In particular, he applied bounded trust region strategies to deal with problems that are overparametrized and likely to have nonunique solutions. Our results with this algorithm, called NTREST (Nonlinear Trust Region Estimation), have shown that these approaches are more reliable than and just as efficient as general-purpose NLP strategies. These are currently being incorporated within a large scale SQP framework as well to take advantage of rapid convergence. This approach is currently being extended to EVM problems as well. Moreover, this algorithm was applied to a challenging parameter estimation problem arising from a polymer reactor model. Applied to a number of cases, Nikhil was able to determine solutions to a variety of poorly conditioned parameter estimation problems. Two reprints that describe this approach are given below.

In a project sponsored by Exxon Upstream Research, Shivakumar Kameswaran has taken over this project and is working on system identification and parameter estimation for oilfield applications. Using IPOPT and AMPL as a dynamic optimization tool he is studying parameter estimation for distributed parameter systems that are potentially ill-conditioned. Here the permeability field needs to be determined using data taken from core samples extracted from reservoirs. Knowledge of this field allows the development of flooding strategies for optimal oil extraction. Moreover, the reservoir model contains a number of interesting features including complementarity relations for capillary pressure and multivariate measurements. Shiva has formulated this problem as a large-scale MPEC and obtained very efficient results. These results have also been validated with actual core data. This is currently being extended to large-scale history matching problems for reservoir models. Also, these models are currently being converted into an AIMMS format and will be solved through the new interface to IPOPT. A reprint of this study is listed below.

Ignacio Grossmann's Group

Algorithms for Nonlinear Disjunctive Programming

Student:	**Nicolas Sawaya [Ph.D., started Jan02]**
Visitor:	**Lorena Bergamini [Ph.D. Jan 03]**
Research collaborator:	**Aldo Vecchietti [Researcher at INGAR]**
New Developments:	**Rigorous approximation for nonlinear convex hull reformulation**
	Branch and bound, OA and hybrid method implementation in open source project

Nicolas Sawaya

The objective of Nick's project is to develop novel solution methods for nonlinear generalized disjunctive programs (GDP). There are two major issues that arise in the continuous relaxation based on the convex hull for linear or nonlinear problems: (a) the corresponding formulations may lead to a problem of large size due to the disaggregation of variables; (b) the corresponding relaxation may produce a lower bound similar or equal to the one obtained from the big-M reformulation of the GDP. A major objective in Nick's work has been to develop effective cutting plane methods for linear GDP problems. The other objective has been to develop an integrated framework for solving nonlinear GDP problems.

The first major step in Nick's research work was to develop a solution method for linear GDP problems that relies on cutting planes, and that can generally be embedded within a branch and cut algorithm. The major steps of the algorithm are to first solve the big-M relaxation. Next, we formulate and solve a separation problem in which we minimize the difference between a feasible point in the convex hull relaxation and the solution of the big-M problem. Here we can use the 1, 2 or infinity norm, 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 this not only tells that the convex hull formulation is tighter, but one can derive a cutting plane, which for the linear case corresponds to a facet of the convex hull. The derivation of successive cutting planes continues until the improvement in the lower bound of the big-M model with the cutting planes lies within a tolerance. The idea is then to switch to a branch and bound method. Nick has developed a nice theoretical derivation of the cutting planes for the 1, 2 and infinity norms based on the use of subgradient optimization. Nick applied his cutting plane technique to three major problems using the infinity norm. The first is 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 largest problem that Nick solved involved 21 rectangles. The convex hull formulation is significantly larger than the big-M model (5272 vs 1072 constraints, 4244 vs 884 continuous variables; both have 840 0-1 variables). The big-M formulation required 1 416 137 nodes and a CPU-time of 4093 with CPLEX 8.1. The convex hull formulation required 968 652 nodes in a time limit of 10 800 secs in which the problem was not solved to even feasibility. In contrast with 60 cutting planes the number of nodes was reduced down to 28611 nodes and 79 seconds! It should be noted that these times include the times for solving the separation problem. Nick also solved 10 process retrofit problem, and extension of a model that Jennifer Jackson formulated, and he also addressed a job-shop scheduling problem with up to 10 jobs and 8 stages. 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 has also investigated the use of cutting planes for solving nonlinear disjunctive problems. He has considered as a first step nonlinear GDP problems that are reformulated as big-M MINLP's and solved through branch and bound. Nick has tested this method on a batch design problem with intermediate storage. The convex hull reformulation involved 1296 constraints, 637 continuous variables and 89 0-1 variables. In contrast the big_m model only involves 800 constraints, 239 continuous variables and 89 0-1 variables. The convex hull formulation was solved in 711 secs enumerating 5 359 nodes. The big-M formulation was solved in 787 secs enumerating 12 449 nodes. The NLP relaxations were 650,401 and 641,763, respectively. With the proposed cutting plane method, using the infinity norm, the NLP relaxation of the big-M was increased to the one of the convex hull with 58 cutting planes. In that way the number of nodes was reduced to 7 528, and the required time to 610 secs (including 8.7 secs for the cut generation). Thus, the proposed cutting plane led to good improvements. Nick plans to unify the application of cutting planes to the different solution methods for GDP

A major issue that we had to revisit is the nagging problem of how to implement the constraint $\lambda\, g(\nu/\lambda)\le 0$ for the case when λ goes to zero and when g is nonlinear and convex. In our previous work we had used the simple approximation $(\lambda+\varepsilon)\, g(\nu/(\lambda+\varepsilon)\le 0$. This however can give rise to problems depending on how ε is selected. The main problem here is that if ε is set too small there are problem with accuracy. If ε is somewhat large then if a disjunct term does not apply and the inequalities are violated it may make the approximation infeasible. Nick has proved that a rigorous approximation that avoids both problems is given by $(\lambda_{jk}+\varepsilon) g_{jk}(\nu_{jk}/(\lambda_{jk}+\varepsilon)) \le \max_{\nu_{jk}\in(0,U_{jk})}(\max\ (\varepsilon g_{jk}(\nu_{jk}/\varepsilon),\ \varepsilon g_{jk}(\nu_{jk}/(1+\varepsilon))))$, 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, $(\lambda_{jk}+\varepsilon) g_{jk}(\nu_{jk}/(\lambda_{jk}+\varepsilon)) \le \max\ (\varepsilon g_{jk}(0),\ \max_{\nu_{jk}\in(0,U_{jk})} \varepsilon g_{jk}(\nu_{jk}/(1+\varepsilon)))$ Nick has successfully tested this approximation scheme in several examples (analytical, process network, safety layout) using values of $10^{-7}\le\varepsilon\le 10^{-4}$. For instance, in the analytical case the value of the objective ranged from 1.169029 for a tolerance 1E-4 to the correct value of 1.171570 for 1 E-7. Interestingly, in all cases all cases convergence was achieved without failure the computational requirements were identical. This work has been written up as a short note and submitted for publication.

Finally, Nick is also helping to build a library of convex MINLP problems that will be used in the CMU-IBM project for an open source code for MINLP that involves Larry Biegler and Gerard Cornjuelos from the Tepper Business School. Nick has created a number of problems related to layout and safety that have proved tobe particularly difficult to solve. The postdoc Pierre Bonami has implemented a branch and bound code that uses IPOPT. He has also completed the implementation of the outer-approximation method as well as hybrid variants of the Quesada and Grossmann LP/NLP based branch and bound. Work is under way to complete a numerical study on a large set of convex MINLP problems that we will report in our next newsletter.

Lorena Bergamini

Lorena, a Ph.D. student from INGAR in Argentina working under the direction of Pio Aguirre and who spent one semester with us, developed a new deterministic algorithm for the global optimization of process networks that are formulated as Generalized Disjunctive Programs and that involve nonconvexities. The global optimization algorithm relies on the use of piecewise MILP approximations (no spatial branch and bound search). Also, the method is based on the Logic-Based Outer Approximation (OA) algorithm developed previously by Metin Turkay and that overcomes difficulties related to singularities that are due to zero flows. The method developed by Lorena is capable of handling nonconvexities, while rigorously guaranteeing the global optimality of the synthesis of process networks. This is accomplished by constructing a master problem that is a valid bounding representation of the original problem, and by solving the NLP subproblems to global optimality. Lorena assumed that the functions involved are sum of convex, bilinear, and concave terms. In order to rigorously maintain the bounding properties of the MILP master problem for nonconvex problems, piecewise linear under and overestimators for bilinear, and concave terms are constructed over a grid with the property of having zero gap in the finite set of points. The set of these approximation points are defined over subdomains defined by bounds of variables and solution points of the previous NLP subproblems. For bilinear terms, the convex envelope by McCormick is used. Disjunctions are used to formulate the convex envelope in each subdomain, and the convex hull of these disjunctions is used to provide the

tightest relaxation. Linear fractional functions are treated in a similar way. Piecewise linear subestimations replace the concave terms. The NLP subproblems are also solved to global optimality using a reduced MILP master problem. Since the NLP subproblems are reduced problems, involving only continuous variables related to a process with fixed structure, the variable bounds can be tightened thereby enhancing the underestimators. Lorena has applied this algorithm on a number of different problems. For instance, the algorithm has been applied in a process network problem that originated in an internship of Sangbum Lee at Eastman Chemical and that involves 17 Boolean variables, 973 continuous variables and 725 constraints. The algorithm required 5 minutes, while BARON could not solve the problem within 15 minutes. Lorena has completed a manuscript on this work which has been accepted for publication.

Aldo Vecchietti: LOGMIP and modeling issues

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 main features of LogMIP are several language constructs in order to concisely formulate GDP problems. The syntax developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. An interesting related development has also been to show that logic constructs that are commonly used in Constrained Logic Programming (CLP), such as implications for constraints (e.g. $g(x) \leq 0 \Rightarrow f(x) \leq 0$) can be systematically converted in the form of disjunctions. The intent is also to be able to accommodate hybrid models that are partly expressed as disjunctions and partly as equations in algebraic form.

Aldo has completed in LogMIP the definition of disjunctions over sets and subsets. The conditional statement operator WITH in conjunction with other operators: relational operators (<, <=, =, >, <=), logical operators (and, or) and sets operators (ord, card, in) or using a subset definition are used to control de disjunction's domain defined over a set. 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 that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. The latter has yielded very impressive numerical results. Aldo found that the big-M formulation of the retrofit planning problem takes about 1745 nodes with OSL, while convex formulation through LOGMIP only requires 9 branch and bound nodes!. For solving nonlinear disjunctive/hybrid problems Aldo has also automated the logic-based OA algorithm by Metin Turkay, which is suitable for nonlinear GDP process network problems. Work is under way to implement the reformulations for nonlinear GDPs. The LogMIP Website is now also available, http://www.ceride.gov.ar/logmip/. The Website includes now some explanation about LogMIP, the User's manual, solvers and examples downloads, references and links.

Modeling of Hybrid Systems and Mixed-integer Programs

New developments: Type Theory for reformulation of GDP into MILP

Students: Ashish Agarwal [Ph.D., started Jan 02]

The initial objective of Ashish's project was to develop a new hybrid systems framework for modeling supply chain networks. The basic idea in Ashish's project has been to rely on a hybrid dynamic systems representation that combines differential equations to capture the continuous dynamics and automata to capture the discrete dynamics. Each automaton describes the space and dynamics of a single discrete variable. The continuous dynamics is used to represent material flow, while the discrete dynamics is used to model scheduling decisions. The hybrid dynamic representation is then applied to a supply-demand network in order to provide a formal representation of the system, determine the optimal operating conditions, scheduling deliveries, selecting between outsourcing and production, and performing a dynamic allocation of resources. Ashish developed a representation based on automata than can be systematically transformed into one with finite states, then to a disjunctive programming model, and finally into a

mixed-integer linear program. In this way an important accomplishment is that one can systematically derive the mixed-integer linear programming model describing the supply demand optimization network problem. Ashish has tested the model formulation on a small supply chain optimization problem demonstrating that the model can be expressed in very compact form. Ashish has completed a manuscript describing this work.

Over the last year, Ashish's research direction has changed. With the collaboration of Professor Bob Harper from Computer Science, he has been investigating the use of Type Theory as a systematic formalism based on logic for proving correctness of formulations for mathematical optimization. The basic idea in type theory is to rigorously define the different variable and operator types using logic constructs to ensure that all transformations of data, variables and equations are "well-formed." In this way one can use such a representation to define mappings as is for instance the case of the reformulation of generalized disjunctive programs to mixed-integer linear programs. Furthermore, one can use type theory as a basis for developing software that has a strong foundation, and that is more likely to be free of errors. Ashish has applied this formalism to generalized disjunctive programming problems for transforming them automatically into MILP models. This has required a sophisticated theoretical development based on type theory that in turn he has used as a basis for software development. Asish has used the language ML for developing the software and has demonstrated the application to several GDP models. Ashish is in the process of finishing his Ph.D. thesis and of writing the corresponding papers.

Optimal Synthesis of Integrated Process Water Systems

New developments: **Global optimization of NLP/MINLP superstructure**

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

Ram's project deals with 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 is 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 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 corresponding model for which no alternatives are considered for the selection of treatment units corresponds to an NLP model with bilinearities in the mixers given by the product of flows times concentrations in ppm of the contaminants. Ram has 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. The physical interpretation is that due to the approximation in the mixers the total mass balances does not hold for each contaminant. These cuts ensure that they do hold. The algorithm also relies on bound tightening and on branching only on the flows. The bisection rule was found to be the most effective for partitioning.

Ram has tested his method with several examples. In one containing 3 process units and 3 treatment units, the corresponding NLP involves 150 variables and 118 constraints (80 bilinear terms). CONOPT failed to solve the NLP from various starting points, and when it converged to a local solution, the best it found had an objective of 138.56 ton/hr (feedwater plus amounts water treated). The method of Ram converged to the global solution of 128.12 ton/hr requiring 7 nodes in the branch and bound tree and 54 secs of CPU-time. BARON was also used to solve this problem requiring 1807 nodes and 454 secs. In another 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. Ram has also extended the model to general cost functions and to variable number of treatment units which gives rise to an

MINLP model due to 0-1 variables that are needed to model these units. For this case Ram has solved a problem involving 2 contaminants, 4 process units and two treatment units, each with the choice of two technologies. Also concave cost functions were used. The size of the MINLP was 4 0-1 variables, 178 continuous variables and 190 constraints. The proposed method required 1 node and 2.3 secs to find the global optimum ($619,205), while BARON required 37621nodes and 17541 secs. DICOPT converged in this case in a suboptimal solution ($ 665,827). Ram has completed a manuscript on this work which has been submitted for publication.

As a next step in his research, Ram has considered the extension of the above problem to the case when the water system is under multiperiod operation in which the loads in the units change as well as the recoveries in the treatment units. One motivation for addressing this problem is to use it as a basis for a two-stage stochastic optimization approach. The difficulty of the global optimization for the multiperiod case is that the corresponding NLP or MINLP becomes much larger. Furthermore, it becomes necessary to introduce 0-1 variables for the piping in order to control the potential complexity in the configurations for each period. Ram has started to explore an algorithm that relies on Lagrangean decomposition. Motivation is to solve the global optimization independently for each time period. He considered a problem with 2 process units and 2 treatment units and 10 time periods. The MINLP model involved 28 0-1 variables, 1428 continuous variables and 1604 constraints. Performing one single iteration led to a gap of only 0.7% requiring 162 secs. Ram intends to concentrate over the next few months on this solution approach.

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: Generation of alternative structures through propositional logic

Students: Mariana Barttfeld (Ph.D. INGAR-graduated August 2003)
Collaborators: Jose Caballero [Associate Prof., Univ. Alicante]

This project deals with a modeling framework for separation systems based on the State-Task Network (STN) and State Equipment Network (SEN) representations. These models are formulated with generalized disjunctive programming (GDP) models that explicitly handle discrete and continuous variables. The intent has been to develop rigorous optimization procedures that can make use of tray by tray models. Mariana Barttfeld from Argentina concentrated on MINLP and GDP models for single columns and complex column configurations. Jose Caballero in Spain is working on the analysis and synthesis of thermally integrated columns.

Mariana Barttfeld

Mariana stayed with Ignacio's group for one year in a collaboration with Prof. Pio Aguirre from INGAR in Argentina. She first performed a comprehensive comparison between MINLP and GDP models for optimal design of distillation columns in which several representation of the superstructure based on tray-by-tray models were used. In all cases the MINLP models took about one order of magnitude longer time than the GDP models. On the other hand the reduction scheme of the MINLP model produced lower cost solutions than with the GDP models due to a strategy for reducing candidate trays from the relaxation. Mariana also investigated the synthesis of superstructures for complex column configurations (e.g. side rectifiers, side strippers) using tray-by-tray models that she studied for individual column design. The superstructure is based on the reversible distillation sequence model by Fonyo (1974) for which Mariana developed both STN and column superstructure representations, for both zeotropic and azeotropic mixtures. For the optimization of the superstructure she developed a decomposition method in which the basic idea is to consider first the selection of column sections, and next the selection of trays for the selected sections. A GDP model was first formulated, which is solved as follows. The NLP thermodynamic initialization is first solved with the maximum number of trays for all sections. This is then used to derive an MILP master problem (based on convex hull) for selecting the sections in the superstructure. This model then selects the sections for which another MILP is formulated for selecting the number of trays in the selected sections. The reduced NLP subproblem is then solved to obtain an upper bound to the cost. An integer cut is added and the corresponding MILPs are updated. These are then solved to generate new configurations based on sections, and number of trays. Mariana solved several problems including an example of an azeotropic mixture (methanol, ethanol, water). in which she used a superstructure with 5 columns. The GDP involved 210 discrete variables and about 10,000 continuous

variables and constraints, and was solved in 64 minutes, yielding a two column configuration with side stripper and side extraction. The work by Mariana was recently presented at a plenary talk at the ESCAPE15 Conference.

Jose Caballero

In the past Jose has addressed the issue of systematically generating all the configurations for thermally coupled distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. Jose developed a set of logic propositions that can be expressed as constraints in an GDP model to define the search space for these thermally integrated columns. Jose also derived equations to calculate the number of thermodynamically equivalent configurations for a given sequence of tasks. Jose has developed a novel superstructure for synthesizing non-azeotropic mixtures with the Underwood-Fenske-Gilliland approximations. The synthesis approach considers alternatives from conventional sequences, in which each final distillation column has a condenser and a reboiler, to fully thermally coupled distillation sequences going through all possible intermediate combinations. In order to perform the optimization of the superstructure Jose formulated the problem as a disjunctive programming problem, and developed a two-stage solution procedure. In the first one a sequence of tasks is optimized, and then in a second stage the best configuration in actual columns is extracted among all the thermodynamically equivalent configurations. The model has proved to be robust and reliable. The more complex example involved 5 alcohols (ethanol, isopropanol, 1-propanol, isobutanol, 1-butanol). The optimal configuration involved 5 columns with 24 trays (AB/BCDE), 45 trays (BCD/E), 40 trays (BC/D), 120 trays (A/B) and (B/C) 29 trays. The CPU-time required was several minutes. Rigorous simulations in HYSYS showed very good agreement with results presented.

In his recent work Jose has been investigating a strategy for determining optimal design of distillation columns using a process simulator (ASPEN) and using the disjunctive programming framework. A major motivation has been to avoid the need of explicitly handling the thermodynamic equations as has been the case in Mariana's work. The idea in Jose's model is to adopt the Logic-Based Outer-Approximation Method in which the NLP subproblem is given only by the existing trays in the column. For this Jose uses the optimization capability in ASPEN to optimize a column with fixed number of trays. In order to define the MILP master problem Jose performs numerical perturbations on the degrees of freedom (usually only two variables). In addition he performs a sequence of simulations by adding and deleting trays in each section in order to evaluate the economic potential of these decisions which are modeled as 0-1 variables in the MILP. This scheme has proved to be quite successful. So far largest problem that Jose applied it was to a mixture of 2-propanol, 1-propanol, i-butanol and 1-butanol. A column with 70 trays was postulated (feed in tray 35). The optimum was found in 3 major iterations. The design yielded a column with 27 trays (tray 24 to 57) and was solved in about 1 min CPU-time. Jose is finishing the testing of this method with few more examples. A manuscript has been written describing this work.

In a recent development Jose looked at the question on how to derive all feasible structures from the superstructure described above that he has embedded from thermally coupled to simple columns. Since Jose has written the logic propositions in Conjunctive Normal Form (CNF)(, this is equivalent to converting these into Disjunctive Normal Form (DNF). The problem is that this transformation is non-trivial. However, Jose considered two possible approaches. One is to pose the CNF logic as a constrained logic programming problem. In this case by using OPL one can in fact generate all solutions to the CNF propositions that are equivalent to each of the clause in DNF form. The other approach is to convert the CNF logic into linear inequalities and pose the problem as an integer program with zero objective. In this case by using BARON one can find all the solutions to the integer program, which again represent each term in the DNF form. The reason this development is significant is that w have now a systematic way of generating the DNF logic for superstructures. Our conjecture is that if we translate this as linear equations (ie each original binary variable is a linear combination of the possible solutions in DNF), this ought to provide a strong constraint that will greatly expedite the branch and bound search. This may be accomplished whether or not the constraint leads to a tighter lowerbound or not. We hope to report on this issue in our next newsletter.

Synthesis of Crystallization Processes

New developments: **Superstructure optimization for refrigeration system**

Post-doctoral fellow: **Carlos Mendez (started Janaury 2003)**

In a joint collaboration project with Jeff Logsdon, John Myers and Scott Roberts from BP, Carlos has been addressing the separation of paraxylene, orthoxylene and methaxylene through a crystallization process given that their boiling points are very close making the use of distillation unattractive. Carlos first developed an NLP optimization model for the operating and design optimization of a fixed configuration of a crystallization process for the separation for paraxylene. The process involves crystallizers, reslurry drums, centrifuges, heat exchangers and a refrigeration system. The model, which makes use of short-cut equations for predicting the mass and energy balances and sizes, and simply assign costs for refrigeration, is quite challenging to converge due to the nonlinearities involved. To circumvent this problem Carlos developed a two-stage procedure the increase the robustness of the convergence. The proposed model has been extended recently as an MINLP model for optimizing the topology of the flowsheet and as well as the operating conditions. The first step involved the optimization of the topology for the crystallizers. This has involved a superstructure that is similar in nature to the Floudas superstructure for heat exchanger networks, except that several exiting streams from the crystallizers that are directed to the others can be eliminated since each crystallizer does not maintain a unique identity as is the case of matches in heat exchanger networks. The results have shown that the predicted structure tends to have fewer crystallizers than the ones used in practice. More recently Carlos has been able to perform the optimization of the entire superstructure considering two and three stages of crystallizers and reslurry drums. The results have indicated that the three stage system may be advantageous since the recycle is significantly reduced for this case.

In order to explicitly include the refrigeration system as part of the optimization of the crystallization process, Carlos has considered a superstructure that is similar in spirit to the one we had developed many years ago in the Ph.D. work of Mark Shelton. At that time temperatures had to be discretized in order to reformulate the problem as an MILP. In this case Carlos has been able to use continuous temperatures which gives rise to an MINLP problem. He has considered a cascaded refrigeration system consisting of two cycles (ethylene and propylene) where the number of stages are optimized. The model relies on a number of short-cut and empirical thermodynamic, efficiency and cost correlations that provide good agreement with real plant data. Carlos has been able to successfully solve this model for fixed loads of the crystallization system. Work is under way to performing a simultaneous optimization of the crystallization and refrigeration system.

Multistage Stochastic Optimization for Design and Planning of Oilfield Infrastructures

New Developments: **Lagrangean-based branch and bound method for solving multistage programs with scenario trees that are decision dependent**

Students: **Vikas Goel (Ph.D. started January 2001)**

Vikas successfully passed his Ph.D. exam and has joined the Upstream Research Center of ExxonMobil in Houston. The specific problem that Vikas has considered in his project is an offshore gas-producing site with a number of reserves of gas, or fields. The size (total recoverable gas from a reserve) and the deliverability (maximum rate of recovery for a reserve) of some of these fields are known with certainty, whereas the rest are uncertain and described by discrete probability distribution functions. Given this information, the problem consists in making investment decisions regarding what fields should be exploited and what infrastructure needs to be set up for this purpose. Operational decisions relate to determining the production rates of the fields over time. Vikas developed a multistage stochastic optimization in which the investment decisions define the structure of the scenario tree. Vikas also generalized the problem for general purpose linear multistage stochastic programming..

Vikas first discovered the interesting point in the gasfield problem that the size and deliverability are "endogenous" parameters rather than "exogeneous" (e.g. prices), which implies that the scenario trees depends of the time when the decisions are made. The implication of this observation is that for endogenous variables, the structure of the tree of scenarios is dependent of when the decisions are made. Based on this fundamental observation, Vikas formulated

the variable scenario tree/multistage optimization problem as a hybrid MILP/GDP problem, where the disjunctions are used to define the structure of the scenario tree. To solve this difficult problem, Vikas first developed an approximate solution technique where the basic idea is to search in the space of scenario trees to find the one that is optimal. The procedure starts by optimizing the problem independently for each scenario, which provides an upper bound to the NPV (wait and see). Next, at every iteration of the algorithm, a specific scenario tree is generated using the solution of the deterministic expected value problem. The multistage stochastic program for the corresponding tree is then solved in order to yield a lower bound. Since this multistage problem can become very large, Vikas used a shrinking horizon approach to avoid the simultaneous solution in the full space. The procedure is continued until the lower and upper bounds lie within a given finite tolerance. The largest problem that Vikas solved involved 4 certain and 2 uncertain fields in 8 years. The number of scenarios was 729. A full space formulation would require more than 4 million 0-1 variables. The approximate solution was solved in about 9 hours of CPU time and had an expected NPV of $79 million, a $5.6 million improvement over a deterministic solution.

Motivated by Vikas' work in the multistage stochastic optimization of gasfield problem, he generalized the scenario decision dependent problem to general linear stochastic programming problems. The interesting contribution by Vikas was that he was able to develop a closed-form disjunctive programming formulation in which the variable structure of tree is handled through disjunctions. This was accomplished by first representing the stochastic problem through disaggregated states at each time period. These are enforced to be the same through "non-anticipative constraints" that ensure that the states be the same when the endogenuous uncertainties are not revealed because no decisions are made. Otherwise, they "explode" into the nodes that define the events in the tree. While the closed form model is conceptually satisfactory, the drawback is that the number of disjunctions is very large since all possible pairs of discrete-states defined by discrete probabilities must be considered. Fortunately, through a very nice and sophisticated proof, Vikas has shown that it is sufficient to consider only successive adjacent pairs which greatly reduce the size of the problem. This has allowed him to solve small problems by transforming the linear disjunctive problem into an MILP with the big-M transformation. For larger problems, however, the resulting MILP is too large. To circumvent this problem Vikas has recently conceptualized a branch and cut method in which the disjunctions are dualized so that the nodes involve a Lagrangean relaxation subproblem which yields stronger lower bounds than the full space 0-1 relaxation. Furthermore, the bounds can also be strengthened with a lot-sizing reformulation. Vikas has applied his theoretical results to a process related problem where two additional processes can be included in a multiperiod network in which there is uncertainty in the yield, whose realization is revealed with a one period delay. For the application of the Lagrangean based branch and bound method he considered a manufacturing problem that has been addressed by Jonsbraten ("sizes problem"). The problem is similar to a lot-sizing problem but also involves manufacturing parts in different sizes. When Vikas' solution method was applied to the largest problem it involved 3,136 0-1 variables, 60,993 continuous variables and 181,939 constraints! This very large problem was solved with the proposed method within 0.038% of optimality in only 3 nodes requiring 13,507 secs (about 3 hours 45 minutes). In contrast, a conventional LP-based branch and bound solved the problem in about 37 hours within 0.3% of optimality and requiring 71,151 nodes. This means that the proposed method produced a better solution in one tenth of the time. The manuscript describing this work has been submitted and accepted in the journal *Mathematical Programming*.

In the last part of his Ph.D. thesis Vikas developed in collaboration with Amr El-Bakry and Eric Mulkayan from ExxonMobil an implementation in C++ of the branch and cut method described above for solving stochastic programs with decision trees that are dependent of design decisions. The goal of this implementation is to have a general computational tool that can be more easily adapted to the solution of a variety of stochastic problems. In this method non-anticipativity constraints are dualized while disjunctions are relaxed. In this way nodes involve a Lagrangean relaxation subproblem that involves the solution of MILP subproblems for each scenario. The advantage of the approach is that it yields stronger lower bounds than the full space 0-1 relaxation. Vikas developed the C++ implementation using an object-oriented modular framework. Major modules include preprocessing, bounding, branching, feasibility generation, and were interfaced with CPLEX. Vikas applied his method to gas field problems that ranged from 3 to 81 scenarios per time period, which in turn gave rise to MILP problems that involved from 594 0-1, 4480 continuous and 7457 constraints to 16,281 0-1, 125,956 continuous and 386,597 constraints. These problems were solved in 169 secs for the smallest and in 37,204 secs (over 10 hours) for the largest. Vikas compared the performance with a direct solution of the MILP using CPLEX. By allowing 10 times the CPU time for Lagrangean relaxation, CPLEX was faster in the smallest problem (49 secs), but in all others it did not terminate in in same cases obtained a solution that was significantly lower in profit (e.g. 71 vs 86). Vikas has produced a manuscript on this work which has been submitted for publication.

Strategies for Reduction of Time-Varying Uncertainty in the Planning of Process Networks

New Developments: **Disjunctive/MILP model**

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

Bora Tarhan, a new Ph.D. student who will follow Vikas' line of work, has been addressing the following stochastic optimization problem. 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 has developed a new mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints. In order to solve this special multi-stage stochastic program he has reformulated it as a mixed-integer linear program, which can be solved through an LP-based branch and bound for smaller instances, or with a special decomposition that is similar to Vikas' Lagrangean branch and bound. Work is under way to test the various solution methods.

Scheduling of Batch and Continuous Multiproduct Plants

New Development: **New RTN models for multistage batch plants with parallel equipment**

Ph.D. student: **Christos Maravelias (finished January 2004; currently at Wisconsin)**

Post-doctoral fellow: **Carlos Mendez (started Janaury 2003)**
Pedro Castro (finished July 2005)

Christos Maravelias

Christos, who currently is a faculty member at the University of Wisconsin, proved as part of his postdoc that his continuous time formulation for the State-Task Network can be reduced to the conventional discrete time formulation of the State-Task-Network when fixed time intervals are used. Although intuitively this is a result that one would expect to hold, it has never been proved before. The derivation of this property is described in a recent manuscript that has been accepted for publication in AIChE Journal. Aside from being of theoretical interest, this opens up the interesting possibility of solving the discrete model with the hybrid MILP/CP approach that Christos has been developing.

Carlos Mendez

In collaboration with Iiro Harjunkoski and Marco Fahl from ABB, and from Jaime Cerda at INTEC, Carlos completed a comprehensive review of the area of batch scheduling. In this paper a general a roadmap is given for classifying the problems as well as the optimization models. The models are then reviewed according to the classification with their main equations from the standpoint of discrete and continuous time STN and RTN models, and from the standpoint of sequential models for multistage plants. Numerical results are presented for discrete and continuous time models for a well-known Kondili example and an industrial size problem proposed by Kallrath from BASF. These results were obtained by our visitors from Barcelona, Anna Bonfill and Gonzalo Guillen. The paper next discusses a series of real world examples to illustrate the considerations that future methods must account for. The paper then reviews academic and industrial research with reference to commercial software. Finally, the paper discusses other solution approaches, the need to use special strategies for large industrial problems, and the area of rescheduling. The manuscript has been submitted for publication. We believe that it should be very useful for those who want to get acquainted with the batch scheduling area.

Perdo Castro

Pedro Castro has completed his stay at Carnegie Mellon. He made important contributions with a continuous RTN model (Resource Task Network) in his Ph.D. in Portugal, and used it as a theme for his research at Carnegie Mellon The RTN is an interesting representation proposed by Pantelides in which the model is viewed as a balance of resources (of equipment, states, utilities, manpower, etc.). Pedro first has examined the single stage problem with parallel lines, a problem that Vipul Jain addressed in his Ph.D. thesis. Pedro was able to reproduce the results of Vipul in the sense that he also found that the computational time in the common MILP and CLP models increases exponentially with problem size, while the hybrid MILP-CP method attains reductions of several orders of magnitude an can solve in very little time the larger instances. He then also found that his continuous time RTN model exhibits exponential behavior. However, he 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 model. He solved problems ranging from 12 orders and 3 units, up to 30 orders and 5 units for the cost minimization case. This was a truly a surprising result because it comes to show again the impact that alternative formulations can have in solving MILP problems. 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 models 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. Pedro also examined the performance when the objective is minimization of earliness. In this case the discrete 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 trend that was also observed is that continuous time models were more effective in small to medium size, while discrete time was better for the larger problems. 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 was submitted for publication.

Finally, Pedro was also involved in a challenging industrial pharmaceutical problem that was supplied to us by ABB through Iiro Harjunkoski and Marco Fahl. This problem had the feature that it is multistage, but with very significant changeover times, and with complex operating rules. Both, 30 and 50 order problems proved to be unsolvable with known existing MILP methods. For this reason, Pedro proposed a heuristic decomposition method that consists of sequentially selecting a subset of orders that are then scheduled recursively in the mode of a "rescheduling" problem in which the given subset is optimized, but the relative sequencing is enforced for previous subsets of orders with start and end times left as free variables. Carlos Mendez also developed a decomposition strategy that is similar in nature but does not require the selection of subsets of orders to be rescheduled. Using such both approaches Pedro and Carlos were able to obtain solutions that are often very close to the global optimum. Work is under way to complete a manuscript on this problem.

Simultaneous Planning and Scheduling of Continuous Multiproduct Plants

New developments: **Development of aggregate and detailed models**

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

Muge's project deals with the simultaneous planning and scheduling of continuous multiproduct plants. The initial objective is to consider the case of a single processor on which a number of products must be produced 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).

To address the scheduling problem described above, Muge has first developed a detailed MILP scheduling model using the concept of slots. This model, while accurate, can only solve problems with few time periods, meaning it 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 is simpler to solve but 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 is 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 first an aggregated LP production planning model, but found that it provides loose upper bounds for the profit and production targets that lead to infeasible schedules. Therefore, she 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. The idea of the supercuts is to eliminate those alternatives that involve a larger number of products that the current assignment. These can be eliminated on the basis of optimality arguments. Likewise the idea of subset cuts is to eliminate subsets of alternatives from the current assignment. These are eliminated on the basis that subsets are considered in the detailed scheduling level since the 1-assignments are treated as upper bounds; only the 0 assignments are fixed. The capacity cuts take into account the potential effect of changeovers in limiting the production. It should also be noted that 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 or on a temporal decomposition scheme.

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. The idea is that in the former case the schedule is forced to produce more products in each time period, and hence is more difficult to solve. She considered 5 products and a time horizon ranging from 4 to 24 weeks. The trends in the results were as follows. In the 4 week problem (120 0-1, 987 continuous, 906 constraints) the proposed method converged to the optimum in 207 secs while the detailed model over the 4 weeks did not terminate the search after 6000 secs (8% gap of bounds) and obtained a suboptimal solution. In the case of low demand the proposed method converged in 4.6 secs versus 525 secs for the simultaneous approach. . In the 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 but found a slightly better solution. Muge has completed a manuscript on this project which has been submitted for publication.

Muge is currently doing an internship at Dow Chemical addressing a simultaneous planning and scheduling problem for batch reactors.

Optimal Scheduling of Refinery Operations

New development: **Paper is under review**
Postdoctoral fellow: **Carlos Mendez (started Jan 2003)**

Carlos worked on a joint collaboration project with Iiro Harjunkoski and Pousga.Kabore from ABB in the area of scheduling of petroleum refinery operations. The major goal was to develop a multiperiod model for optimizing the production planning and blending operations in a refinery. The specific problem is to consider a set of product demands over a specified time period for which one has to determine what intermediate products should be allocated to what blender at what time period. Carlos developed a novel recursive LP model for blending that is based on the idea of formulating volumetric and gravimetric properties with linear constraints, while computing the mismatch of

the nonlinear properties with linear approximations, from which a correction factor is inferred for the LP model. This correction is applied recursively, and convergence to good solutions is typically very fast (e.g. 3 iterations). This LP model is then incorporated as part of the MILP scheduling problem where decisions are made for the allocation of blenders and tanks, timing of operations, and amounts of products to be produced and their quality for the given specifications. Carlos developed both discrete and continuous time MILP scheduling models. In this way, extending the solution method for blending, the simultaneous scheduling and blending problem is optimized by recursively solving either of the two MILP scheduling models that incorporate the linear approximations for the blending equations.

The proposed method has been tested with several gasoline mixtures involving 9 components and 12 properties (4 of them nonlinear). The proposed method yields approximations that are very close to the nonlinear model. For problems involving 8 days of operation, 3 blend headers, 12 storage tanks and 3 final products, the proposed method was able to predict solutions with significant improvements in the profit compared to sequential procedures where the blending and scheduling problem are decoupled. The computational cost of the recursive MILP is very small (under 1 minute of computation). The manuscript of this work has been submitted and is currently under revision. An important issue has been the theoretical justification for the convergence, as well as numerical comparison with NLP and MINLP solvers. Our preliminary results indicate that the method is guaranteed to converge to at least a local solution, and that its performance is usually more robust than NLP or MINLP solvers. We will report on our definite findings on these issues in the next newsletter.

Optimization Approaches for Metabolic Engineering

New developments: **Selection of screening strategies for NMR analytes with Analytical Hierarchical Process**

Student: **Soumitra Ghosh (Ph.D., started Jan 02) (supervised jointly with Mike Domach)**

This project on metabolic engineering by Soumitra Ghosh is in collaboration with Mike Domach. The first part of Soumitra's work involved the development of a software package for systematically identifying all the alternate optima that arises in the LP problem for maximizing yield in metabolic networks. The methods he implemented were a recursive MILP method that was developed by Sangbum Lee and a depth-first enumeration method. These methods can provide information on product yield horizons and the optimal "target" values of fluxes to achieve in metabolic networks. These methods can also elucidate the metabolite trafficking possibilities in tissues. While methods that enumerate flux scenarios are useful for the "front-end" analysis of metabolic engineering problems or probing the possibilities in tissue physiology, the evaluation of actual data from a tissue or engineered cells is ultimately needed to verify the veracity of theoretical predictions and mechanistic hypotheses. This gives rise to an inverse problem in which NMR data are used to best fit a linear combination of fluxes that minimizes a sum of squares deviation. However, this nonlinear programming problem is problematic because it is highly non-convex due to the bi-linear and tri-linear terms that arise in the isotopomer distribution vectors. Therefore, in order to obtain reliable results, it is imperative to solve the NLP to global optimality. For this purpose Soumitra has developed a formulation that involves using the results of the "front-end" analysis (MILP solutions) to provide tight bounds in the global optimization of the inverse-problem of data-to-fluxes. Soumitra has applied the code BARON by Nick Sahinidis for deterministic global optimization and obtained good results. He first applied it in a small hypothetical problem in which BARON only required 2.3 seconds to find the global optimum. The problem involved 51 variables and 47 constraints. He then considered an E. coli bacterial mutant that has had pyruvate kinase activity deleted with 17 reversible reactions. The problem involved 910 variables and 897 constraints, and was solved by BARON in about 3 hours. It should also be noted that linking flux distribution forecasting with spectra-to-fluxes calculations provides a potential means for assessing the utility of different analyte sets for ascertaining the net values of metabolic fluxes. Such linked tools may assist in forecasting physiological possibilities in metabolic engineering and in tissue studies as well as help with closing the loop between physiological reality and the system "model" the investigator has conceived.

Soumitra has recently developed a two-tiered computational approach for screening NMR analyte sets for their ability to report on metabolic fluxes. After obtaining the flux bounds via MILP, analytes are first screened for the ability of their NMR spectra to differentiate between different extreme point (or linear combinations of extreme

point) flux solutions. Then, the analytes are screened for whether they provide unique flux values or multiple flux solutions – this is achieved via determination of possible multiple global solutions of the inverse optimization problem. The effect of noise in NMR data is also being considered as a factor in the ability of an analyte set to faithfully provide a correct flux solution as opposed to an alternative solution. The screening strategies have been successfully implemented in a small hypothetical problem and in the E. coli system. An additional aspect that Soumitra has considered is the sensitivity problem of the inferred metabolic pathway with noise measurements in the NMR spectra. His has formulated this problem as an NLP problem to determine the maximum of the minimum deviations in the different peaks of the spectra given that the pathway fluxes lie within a given tolerance. With this additional measure and economic considerations of analyte selection that is driven by the material and labor costs associated with their isolation, there are different trade-offs that one can consider in the selection of the analytes. In order to address this problem Soumitra has applied the Analytic Hierarchy Process or AHP by Saaty. In simple terms the AHP leads from simple pairwise comparison judgments to the priorities in the hierarchy. Soumitra considered the performance of each NMR analyte according to the following criteria: (i) extreme point comparison (ii) abundance data based on both cytosolic content and frequency in proteins , (iii) Multiple Global Optima Test. Glutamate ranked first overall, followed by Alanine, and OAA (aspartate). This ranking was consistent with the results of the structured methodology used in this work. Soumitra is currently completing a manuscript on this work.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: Gabriela Garcia (started March 2000)

Gabriela Garcia has developed web interfaces that are available in:
http://newton.cheme.cmu.edu/interfaces

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 MILPmultiperiod model for utility plants (Iyer)
PRODEV MILP model for scheduling of tests in new product development (Schmidt, Najimas)
MILP for resource scheduling in new product development (Jain, Maravelias)

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

Steinar Hauan's Group

Agent Systems in Engineering Design and Optimization

Students: John Siirola (Ph.D., completed May 2005), and Israel Owusu (Ph.D., 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

John spent the last few months of his thesis to study the impact of algorithmic collaboration in MILP systems using branch and bound (B&B). In principle, B&B should be ideally suited for a distributed approach: any time a particular agent obtains a new best integer solution, it could be shared with the other computational threads and thus used to prune branches in the search tree with greater efficiency. Specifically, we implemented an MIP agent that shares incumbent solutions between CPlex instances using their published method for external heuristic callbacks. We then set up to the agent system to run multiple parallel copies of CPlex -- each configured to use different preferences in their B&B exploration strategy – and compared with the performance of individual instances of CPlex. It is important to note that when these comparisons, we must carefully distinguish between the two fundamentally different goals of the MIP solution process: (a) the time required to identify the optimal solution, and, (b) the time it takes to prove it optimal. It is clear that the agent system is best suited to assist in the first step as proving optimality in principle requires visiting (or pruning) every branch in the search tree.

The results from running CPlex agents on their own were interesting: On average, the performance of randomly generated -- fairly large -- assignment problems were substantially better in a collaborative environment: Speedup factors for identifying the optimal solutions were found to be in the range 8-20 when using 5 CPLex instances compared to individual runs. This includes the case where CPlex is using its internal default settings. However, it is possible to tune CPlex on its own to perform similar to -- or even moderately better -- than the agent system. Furthermore, the total time required to prove solution optimality is was not substantially affected.

We next added CPlex agents to the agent system, i.e. attempted to solve the problem using not only direct B&B solvers, but also a polymorphic model formulation and the complete set of other agents available. The results were very encouraging: On problem sizes where CPlex on its own spends 8 or more CPU hrs to identify the optimal solution and fails to prove optimality in 24 CPU hrs, the agent system -- running on 20 CPUs -- on average identified the optimal solution in less than 10 minutes.

On the application side, Israel has implemented a distributed planning and scheduling model that considers N independent plans -- each with numerous internal processes and M common external products – that experience a single set of demands for each product. While the scheduling for each plant with a given set of production targets are independent, the planning stage requires a policy for assigning production levels to each plant; a non-obvious task in light of the computational complexity of the underlying models. The system is currently set up so we can solve the multi-plant model simultaneously given enough CPU time. Consequently, we can get a quantitative measurement of the best possible solution in the case of perfectly accurate information and product distribution policies. We are currently exploring different strategies for demand allocation as well as information sharing at different time horizons.

Microscale Chemical Synthesis and Sensing

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

(a) 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,

(b) 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,

(c) improved safety as the small amount of materials and energy present significantly reduces the potential impact of accidents and spill,

(d) 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

(e) 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 (Ph.D., started Jan 2002) and Xiang He (Ph.D., started Jun 2003)

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

BACKGROUND

Microfabrication process 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

Anton spent most of the spring semester on automated design of multiplexed chips for electrokinetically controlled separation tasks. This involves both the detailed performance and relative placement of each separation as well as the routing of i/o channels connecting each internal subsystem to fluidic wells on the edge of the chip. The solution process involves iterative solving a set of non-convex NLP problems coupled with 2 NP-hard integer problems. It should be noted that each subproblem is automatically generated and solved by the outer "design logic" and, while the theoretical time complexity of the algorithms used is exponential, we can now achieve complete designs with 10-15 subsystems in less than an hour of computer time.

The units used in these subsystems are all based on separation only. We next aim to extend the algorithms to chips that combine the full range of Lab-on-a-Chip "unit operations" on a single chip. In our collaborative group, we have developed a full set of reduced order (non-PDE) models for all these elementary operations and need to implement the equivalence of a "flowsheet simulator" to evaluate the performance of arbitrary unit sequences. The conceptual development and prototype implementation has been completed by Anton using techniques known from chemical process flowsheet design. We have adapted a standard set of interface parameters for a generic process unit and have packaged the unit-specific physiochemical models in a modular fashion. The complete Lab-on-a-Chip is configured as a connected graph -- known as a "netlist" in the ECE literature -- and solved in two stages. We first obtain the (electrical) driving forces for each of the stages in the dynamic problem by solving a sequence of resistivity network models. Subsequently, the electrical potentials and associated currents are sent to the unit operation modules that calculates the performance of each

A main task for both Anton and Xiang over the next few months will be to test the implementation and integration of the system simulator and its associated unit operations on a range of practical Lab-on-a-Chip systems.

(b) A MEMS-based Gravimetric Biosensor

Students: Michael Bartkovsky (Ph.D., started Jan 2002), Jane Valentine (Ph.D., started Jan 2003),

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

BACKGROUND

This work aims at 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

A fourth generation chip was submitted for fabrication in January of 2005 and returned to us in late April. Unlike previous generation chips, this device appears to have all its onboard transduction circuitry and signaling logic in order; Mike and Anna have basically spent most of the last 6 months learning how to use all the characterization and testing equipment in the ECE MEMS lab and going through all the mechanical and electrical testing of each part of both the 3rd and 4th generation chip designs. However, it now does appear to work and we are able to perform direct differential measurement of vibrations of the basic CMOS structures. The next step will be to turn the metal mesh structures into a membrane by conformal coating with polystyrene and repeat the vibrational measurements. At that point, we will finally be able to test operation in liquid; first without – but hopefully shortly thereafter -- with the presence of chemical binding groups on the membrane surface.

Jane is working on algorithmic approaches to optimal design of sensing arrays based on these MEMS membranes. She has so far completed a reduced order model based on perturbation analysis that allows us to accurately assess the impact of chemical binding to only a part of the membrane surface. These patches allows for a single membrane to become a sensor array in itself; the next step is to use this model in an optimization formulation that aims to determine how to best place N patches on a single membrane to best detect K different targets in the same analytical sample.

Design of Multiproduct Reactive Separation Plans

Students: Scott Turnberg (Ph.D., starting 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 started his work in Jan of 2005 and has spent most of his time so far becoming familiar with the tools for feasibility analysis originally developed by Warren Hoffmaster (PhD 2004). He has implemented a mex interface to the bifurcation/continuation software package Auto2000 to assist in tracking geometric features such as separation boundaries as well as reactive and non-reactive pinch point curves.

Erik Ydstie's Group

Modeling and Control of Particulate Processes

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

This research addresses modeling and control of yield and size distribution in particulate processes. We use a novel method of solar-grade silicon production, the thermal decomposition of saline 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.

In the future, we will link the current size distribution model to a model for gas-solid fluidization to better represent the system. We will also extend the model to include a better representation of the effect of nucleation. The improved model will be used to develop control of the gas and solid flows in the reactor as well as the silicon yield. To address control of this model and particulate processes in general, we will establish required state and parameter estimators. We will also check the generality of our methods on a different particulate process such as the production and growth of biological cells or atmospheric aerosols.

Modeling and Control of Distributed Process Networks

Student: Kendell Jillson (Ph.D.)

We introduce a novel modeling framework for studying dynamics, distributed control, and optimization of complex chemical process networks. We are interested in developing self-organizing structures 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 and basic conservation principles, a multi-component analogy to Tellegen's Theorem of electrical circuit theory was produced. Using this result and passivity theory, a network is shown under certain conditions to converge to a stationary solution when the flow relationships are positive. Also, under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized.

We wrote a conference paper dealing with the passivity and optimality conditions of a general process network. This paper was accepted, and Kendell presented this work in July at the 16th IFAC World Congress in Prague. We are also continuing to write a more extensive paper to submit for publication.

We plan to continue theoretical work in areas of stability, control, and optimization of process networks. We have also begun to develop a networked model of the biological process of angiogenesis, the growth of new blood vessels. This is often signaled by cancerous tumor cells as a way for tumors to increase their uptake of nutrients from the body as they grow. By modeling this problem with our network framework, we hope to gain insight into the system and eventually be able to suggest an optimal treatment strategy for dealing with tumor growth.

Real Time Optimization by Extremum Seeking Control

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

We have developed an online optimization technique for unconstrained optimization based on extremum seeking control. The optimization algorithm behaves as a stand-alone module using existing process models to gather information and adaptively drives the process to its extremum without altering the simulation code. The optimizer uses a second order approximation to a high order system and takes a set of modified equality constraints constructed so that they have the same geometric characteristics of the true steady-state behavior of the process. The module employs a dynamic model to obtain a steady-state model of the system. The steady-state model is then used

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

Passivity Based Control of Multi-Phase Reactor Systems

Student: Yiuan Xu (Ph.D.)

Passivity Based Control of Multi-Phase Reactor Systems

Student: Yuan Xu (Ph.D.)

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.

PUBLICATIONS:

B-05-01
Hong, W., P. Li, G. Wozny, L. T. Biegler, S. Wang, "A Quasi-Sequential Approach to Large-Scale Dynamic Optimization Problems," *AIChE Journal*, accepted for publication (2004) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-02
Laird, C. D., L. T. Biegler and B. V. Bloemen Waanders, "A Mixed Integer Approach for Obtaining Unique Solutions in Source Inversion of Drinking Water Networks," submitted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-03
Kameswaram, S. and L. T. Biegler, "Convergence Rates for Direct Transcription of Optimal Control Problems Using Collocation at Radau Points," submitted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-04
Kameswaran, S., and L. T. Biegler, "Convergence Rates for Direct Transcription of Optimal Control Problems with Final-time Equality Constraints using Collocation at Radau Points," submitted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-05
Arrieta-Camacho, J. J. and L. T. Biegler, "Real Time Optimal Guidance of Low-Thrust Spacecraft: An Application of Nonlinear Model Predictive Control," submitted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-06
Kawajiri, Y. and L. T. Biegler, "Optimization Strategies for Simulated Moving Bed and PowerFeed Processes," submitted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-07
J. R. Perez-Correa and L. T. Biegler, "Nonlinear Dynamic Data Reconciliation Using General Optimization Solvers within Matlab," Proceedings of IMAACA '2005, to appear (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-08
V. de la Torre, V. G. Fox, J. A. Bandoni and L. T. Biegler, "Model Predictive Controller for Periodic Adsorption Processes," Proceedings of *ENPROMER 2005*, accepted for publication (2005) http://dynopt.cheme.cmu.edu/papers/papers.html

B-05-09
Lang, Y-D., and L. T. Biegler, "The IPOPT Interface to CAPE-OPEN," http://dynopt.cheme.cmu.edu/papers/papers.html

G-05-01
Castro, P.M. and I.E. Grossmann, "A New Continuous-time MILP Model for the Short-Term Scheduling of Multi Stage Batch Plants," submitted for publication (2005). http://egon.cheme.cmu.edu/Papers/CastroGrossmannMultistage.pdf

G-05-02
Castro, P.M. and I.E. Grossmann, "An Efficient MILP Model for the Short-Term Scheduling of Single Stage Batch Plants," submitted for publication (2005). http://egon.cheme.cmu.edu/Papers/SingleStagePedro.pdf

G-05-03
Erdirik, M. and I.E. Grossmann, "A Decomposition Method for the Simultaneous Planning and Scheduling of Single Stage Continuous Multiproduct Plants," submitted for publication.

G-05-04
Karuppiah, R. and I.E. Grossmann, "Global Optimization for the Synthesis of Integrated Water Systems in Chemical Processes," submitted for publication. http://egon.cheme.cmu.edu/Papers/PaperKaruppiahGrossmann.pdf

G-05-05
Méndez, C.A., J. Cerdá , I. E. Grossmann, I. Harjunkoski, and M. Fahl, "State-Of-The-Art Review of Optimization Methods for Short-Term Scheduling of Batch Processes," submitted for publication (2005). http://egon.cheme.cmu.edu/Papers/BatchReviewMendezGrossmann.pdf

G-05-06
Sawaya, N.W and I.E. GROSSMANN, "Computational Implementation of Non-Linear Convex Hull Reformulation," submitted for publication. http://egon.cheme.cmu.edu/Papers/ShortNoteSawayaGrossmann.pdf

H-05-01
Hoffmaster, Warren W. and Steinar Hauan. "Using Feasible Regions to Design and Optimize Reactive Distillation Columns with Ideal VLE", submitted to *AIChE J*., June 2005.

H-05-02

Pfeiffer, Anton J., Tamal Mukherjee and Steinar Hauan, "Synthesis of Multiplexed Biofluidic Microchips," accepted for publication in *IEEE Transaction on Computer-Aided Design of Integrated Circuits and Systems: Special Issue on Design Automation Tools for Microfluidic-based Biochips*, Jun 2005.

H-05-03
Siirola, John D. and Steinar Hauan, "Polymorphic Optimization," submitted to *Comp.Chem.Engng*., May 2005.

Y-05-01
Dozel-Mejorada and B. Erik Ydstie, "Input Output Optimal Control of Multi-Scale Systems using Adaptive Policy Iteration," will be presented at the 2005 Annual *AIChE* Meeting, Cincinnati, OH.

REPRINTS

Bizet, Veronique, I.E. Grossmann and Nikola M. Juhasz, "Optimal Production and Scheduling of a Process with Decaying Catalyst," *AIChE J*., 51, 3, pp. 909-921 (2005).

Caballero, J.A., D.Milán-Yañez and I.E. Grossmann, "Optimal Synthesis of Distillation Columns: Integration of Process Simulators in a Disjunctive Programming Environment," Proceedings ESCAPE-15, *Elsevier B.V*., pp.715-720, Barcelona, Spain (2005).

Flores-Tlacuahuac, A., L. T. Biegler and E. Saldivar-Guerra, "Dynamic Optimization of HIPS Open-Loop Unstable Polymerization Reactors," *I & EC Research*, 44, 8, pp. 2659-2674 (2005).

Ghosh, S., T. Zhu, I.E. Grossmann, M.M. Ataai and M.M. Domach, "Closing the Loop between Feasible Flux Scenario Identification for Construct Evaluation and Resolution of Realized Fluxes via NMR," *Computers and Chemical Engineering*, 29, 459-466 (2005).

Goel, V. and I. E. Grossmann, "A Lagrangean Duality Based Branch and Bound for Solving Linear Stochastic Programs with Decision Dependent Uncertainty," Proceedings ESCAPE-15, *Elsevier B.V*. 55-60 Barcelona, Spain (2005). http://egon.cheme.cmu.edu/Papers/EscapeGoelGrossmann.pdf

Grossmann, I.E., Pio A. Aguirre and Mariana Barttfeld, "Optimal Synthesis of Complex Distillation Columns using Rigorous Models," *Computers and Chemical Engineering*, 29, pp. 1203-1215, (2005).

Grossmann, I.E., "Enterprise-wide Optimization: A New Frontier in Process Systems Engineering," *AIChE Journal*, 51, 1846-1857 (2005). http://egon.cheme.cmu.edu/Papers/GrossmannEWO.pdf

Kameswaran, S., G. Staus and L. T. Biegler, "Parameter Estimation of Core Flood and Reservoir Models," *Computers and Chemical Engineering*, 29, 8, pp. 1787-1800 (2005).

Knaebel, S., D-H Ko and L. T. Biegler, "Simulation and Optimization of a Pressure Swing Adsorption System: Recovering Hydrogen from Methane," *Adsorption*, 11, pp. 615-620 (2005).

Laird, C. D., L. T. Biegler, B. van Bloemen Waanders, R. A. Bartlett, "Time Dependent Contaminant Source Determination for Municipal Water Networks Using Large Scale Optimization," *ASCE Journal of Water Resource Management and Planning,* 131, 2, p. 125 (2005).

Lang, Y-D., and L. T. Biegler, "Large-scale Nonlinear Programming with a CAPE-OPEN Compliant Interface," *Chemical Engineering Research and Design (Trans. IChemE, Part A),* 83, pp. 718-723 (2005).

Mendez, C.A., J. Myers, S. Roberts, J. Logsdon, A. Vaia and I. E. Grossmann, "MINLP Model for Synthesis of Paraxylene Separation Processes Based on Crystallization Technology," Proceedings ESCAPE-15, *Elsevier B.V.*, pp. 829-834, Barcelona, Spain (2005). http://egon.cheme.cmu.edu/Papers/PD-051MendezGrossmann.pdf

Raghunathan, A. U. and Lorenz T. Biegler, "Interior Point Methods for Mathematical Programs with Complementarity Constraints (MPCCs)," *SIAM J. Optimization,* 15, 3, pp. 720-750 (2005).

San Román, M.F., E. Bringas, I. Ortiz and I. E. Grossmann, "Optimal Synthesis of an Emulsion Pertraction Process for the Removal of Pollutant Anions in Industrial Wastewater Systems," Proceedings ESCAPE-15, *Elsevier B.V.* pp.649-654, Barcelona, Spain (2005).

Xu, C., P. M. Follmann, L. T. Biegler and M. S. Jhon, "Numerical Simulation and Optimization of a Direct Methanol Fuel Cell" *Computers and Chemical Engineering,* 29, 8, pp, 1849-1860 (2005).