



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

New Directions for Process Systems Engineering

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

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

December, 2003

TABLE OF CONTENTS

General News	3
Executive Summary	5
Status of Research Projects	
<u>Larry Biegler's Group</u>	
<i>General Frameworks for Large Scale Optimization Strategies and Applications</i>	7
<i>Barrier (Interior Point) Methods for Nonlinear Programming</i>	8
<i>Mathematical Programs with Equilibrium Constraints (MPECS)</i>	8
<i>Simultaneous Optimization of Differential-Algebraic (DAE) System</i>	9
<i>Dynamic Optimization for Aircraft Conflict Resolution</i>	11
<i>Large-Scale Optimization for Fuel Cell Models</i>	11
<i>Optimization and Control of Pressure Swing Adsorption Systems</i>	12
<i>Data Reconciliation for Steady State and Dynamic Processes</i>	13
<u>Ignacio Grossmann's Group</u>	
<i>Algorithms for Nonlinear Disjunctive Programming</i>	13
<i>Modeling and Optimization of Hybrid Systems for Supply Chain Problems</i>	17
<i>Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis</i>	17
<i>Synthesis of Crystallization Processes</i>	18
<i>Multistage Stochastic Optimization for Design and Planning of Oilfield Infrastructures</i>	19
<i>Scheduling of Batch and Continuous Multiproduct Plants</i>	20
<i>Optimal Scheduling of Refinery Operations</i>	21
<i>Integration of Product Testing and Planning of Batch Manufacturing Facilities</i>	
<i>Optimization Approaches for Metabolic Engineering</i>	24
<i>Optimal Multiperiod Planning for Catalyst Replacement</i>	24
<i>Software for MINLP Optimization in Design and Scheduling</i>	25
<u>Steinar Hauan's Group</u>	
<i>Feasibility and Economics of Reactive Separation Systems</i>	26
<i>Agent Systems in Engineering Design and Optimization</i>	28
<i>Microscale Chemical Synthesis and Sensing</i>	31
<i>Microscale Total Analysis Systems</i>	31
<i>A MEMS-based Gravimetric Biosensor</i>	32
<u>Erik Ydstie's Group</u>	
<i>Distributed Simulation and Control of Process Networks</i>	33
<i>Adaptive Enterprise Systems</i>	33
<i>Modeling and Control Complex Chemical Reactors</i>	34
<i>Modeling and Control of Particulate Processes</i>	34
<i>Thermodynamics and Process Networks</i>	35
<i>Real Optimization of Silicon Reactors</i>	35
<u>Publications and Reprints</u>	36

GENERAL NEWS

Ignacio Grossmann has completed the first part of his sabbatical leave in Spain as a Fulbright Senior Lecturer at the University of Cantabria in Santander. The second part (February-May) he will spend at ETH in Zürich with the group of Manfred Morari (Insitut für Automatik). Finally, he will spend a few weeks in London at Imperial College.

Ignacio received the INFORMS Computing Society Prize at the Annual Meeting in Atlanta. He also gave the 10th Roger Sargent Lecture at Imperial College on December 4, 2003, “*Future and Scope of Mathematical Programming in Process Systems Engineering.*”

Erik Ydstie finished his work with PPG on the development of a new control system for the PPG windshield forming line in Evansville Ill. He developed a hybrid model represented of the switched system in MATLAB and designed a novel control system in conjunction with PPG engineers. The system was turned on in July and has resulted in significant improvements in yield for both the production line. The pay-back period for this investment in improved control is calculated to be about four months. He is currently working on developing a new control system for the windshield line at the Creighton Plant in PA. This is a continuous leer and the control design philosophy is quite different form the one developed at the Evansville Plant. Erik also concluded his Expert Witness agreement with CA in San Francisco. The case ended up being settled outside court. Vianey and Dimitrios continued working on the Alcoa carbothermic aluminum process. The project is now going into pilot plant testing and the models we developed are being used for preliminary deign studies.

Congratulations to Marta who has taken a job with Norsk Hydro in Norway. She will visit us again in January after she has finished her PhD defense in Norway.

Nicolas Sawaya received the The Geoffery D. Parfitt Memorial Award for his presentation “*A Cutting Plane Method for Solving Generalized Disjunctive Programming Problem*” at the 25th CHEGSA Symposium. Veronique Bizet, visitor from France working with Ignacio, received an honorable mention as the best poster from the CAST Division for the paper “*Optimization Model for the Production and Scheduling of Catalyst Changeovers in a Process with Decaying Performance*” by Bizet, V.M., N. Juhasz and I.E. Grossmann.

We welcome the following new Ph.D. students to the PSE family. Yoshi Kawajiri from Kansai University will be working with **Larry Biegler**. Ramkumar Ruppiah from IIT Dehli and Muge Erdirik from Bogazici University will be working with **Ignacio Grossmann**. Muge will be working in the area of planning and scheduling. Ram will be working in the area of synthesis of integrated water systems. Eduardo Dozal from Texas A&M University and Stephen Craig, also from Texas A&M will be working with **Erik Ydstie**.

PSE 2003

Prof. Bingzhen Chen (Tsinghua University, Beijing, P.R.China) and **Art Westerberg** are co-Chairs of PSE 2003 (<http://pse2003.chemeng.tsinghua.edu.cn/>), the eighth in the triennial series of international symposia on process systems engineering initiated in 1982. The PSE 2003 meeting, which will take place in Kunming, Yunnan Province, P.R.China, will open with a reception on Monday evening, January 5, 2004 and will close at noon on Saturday, January 10, 2004. . The purpose of PSE meetings is to bring together the worldwide PSE community of researchers and practitioners who are involved in the creation and application of computing based methodologies for planning, design, operation, control, and maintenance of chemical processes. The special focus of pse2003 meeting is on the topic of how these PSE methods and tools can support the high-level business decisions required in the process industries. We hope that many of you will be able to attend. We expect it to be a meeting that helps define a future focus for PSE research.

2004 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on March 8-9, 2004. 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 extremely positive. If you have any additional thoughts or suggestions, please let us know.

SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* will be offered on April 29 – May 5, 2004. In the past we were very pleased with the outcome of this course. We had 13 attendees from around the world, both from industry and academia. Also, the course has been extensively revised and includes the following modules:

- a) Conceptual Design - taught on Thursday and Friday (April 29-April 30), with focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.
- b) Optimization - taught on Saturday and Monday (May 1 and 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 Tuesday and Wednesday (May 4-5), 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 McIltrout at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

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://www.cheme.cmu.edu/research/capd/>. This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Other websites of interest are Ignacio's <http://egon.cheme.cmu.edu>, and Larry's <http://dynopt.cheme.cmu.edu>. 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> a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada and Chile. Mexico's will be added soon.

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:

- **Multi-bed Pressure Swing Adsorption (PSA)** processes were optimized for high purity hydrogen separations. This approach improved the recovery of hydrogen from a five bed, eleven step process to nearly 90% with a purity level of 10 ppm CO.
- **Industrial polymerization reactor** was optimized for dynamic operation. The reactor has a number of ill-conditioned characteristics and the optimization was performed in less than 25% of the time of competing methods.
- **Conflict resolution strategies were developed for multiple aircraft.** This approach requires the solution of nonconvex optimization problems. Efficient NLP strategies were applied so that multiple aircraft avoid conflict with each other as well as imposed stationary obstacles with minimum fuel consumption.
- **Source inversions problem in municipal water networks were solved.** This approach is based on a novel NLP formulation applied to large sets of delay differential equations. A number of large-scale systems were considered in order to detect attacks on the network. Problems with hundreds of thousands of variables could be solved within only a few CPU seconds.

Enabling Software From Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the reduced Hessian SQP (rSQP) strategy along several directions. The rSQP strategy has been used for optimization of PDE based models involving convection and diffusion. Examples of this include CVD reactors (**Greg Itle**), PSA systems (**Ling Jiang** and **Vanesa de la Torre**) as well as fuel cell systems (**Cong Xu**). **Andreas Waechter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, called IPOPT, based on many of these SQP concepts. This has 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; more information on downloading and distribution is given below. The IPOPT strategy has spawned exciting applications to challenging problems in process engineering. First, **Arvind Raghunathan** is extending the IPOPT algorithm to deal with Mathematical Programs with Equilibrium Constraints (MPECs); these arise frequently in many engineering systems. In addition, **Maame Poku** is applying IPOPT, its extensions to MPECs, and its AMPL interface, to blending problems. Finally, **Roscoe Bartlett**, now at Sandia National Labs, has developed a comprehensive suite of optimization routines called rSQP++. Written in C++ with numerical routines in FORTRAN, this suite was demonstrated on a wide variety of optimization applications. rSQP++ will be available under Open Source software licenses and more information on distribution will be in the next newsletter. In a new project, **Carl Laird** is extending the work of Roscoe by incorporating the IPOPT algorithm as well as large-scale extensions into rSQP++.

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 has been enhanced further by incorporating the ESO CAPE-OPEN modeling standards currently used in gProms. In a parallel effort, we are working with researchers **Tobias Jockenhoewel** from the Technical University of Berlin is currently completing his thesis on the OCC package, which incorporates these dynamic optimization strategies using MATLAB interfaces. Moreover, **Shivakumar Kameswaran** is expanding the work on dynamic real-time optimization using OCC and AMPL for singular control problems, as well as deriving theoretical properties of this approach.. Finally, **Nikhil Arora** has applied trust region methods for data reconciliation, gross error detection and EVM problems. A trust region code, called NTREST is being refined and is planned to be available for future release.

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

In the area of optimization **Nicolas Sawaya** has derived the theory of cutting plane techniques for linear disjunctive programming in terms of subgradient optimization, and tested the method on a small retrofit design problem that Jennifer Jackson considered in her Ph.D., work. **Lorena Bergamini** has almost completed the paper on the new method for the global optimization for the logic-based OA method. **Aldo Vecchiotti**, has continued expanding capabilities in LOGMIP <http://www.ceride.gov.ar/logmip/>, a GAMS-based code for disjunctive programming. **Ashish Agrawal** has continued in the work related to hybrid systems for supply chain optimization that relies on the use of automata, and has tested his model on a small supply chain optimization problem and on a State-Task network example.

In the area of process synthesis **Carlos Mendez** has been working on a joint collaboration project with BP 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 applying global optimization techniques in the development of an integrated framework for determining intracellular fluxes in a metabolic network along with the design of efficient Nuclear Magnetic Resonance (NMR) experiments for validation purposes. **Jose Caballero** in Alicante is developing a hybrid STN/SEN superstructure for synthesizing thermally coupled columns using short-cut models.

Vikas Goel has applied a multistage stochastic optimization in which the scenario trees are dependent of the design decision to a small process planning problem that was presented at the AIChE meeting. He has also completed the theoretical analysis of the closed-form disjunctive optimization model, and is starting to develop a branch and cut framework that can be applied to a variety of problems. **Christos Maravelias** has completed writing the paper on a novel hybrid MILP/CP strategy for solving continuous-time STN problems with alternative objectives (profit maximization, makespan minimization). He has also been able to apply this method to special cases including single-stage plants with parallel units and multistage batch plants. He has also completed the manuscript where he extended the MILP scheduling model for new product development for the case when investment in resources are considered. **Carlos Mendez** has been developing a novel scheduling refinery MILP model that has the capability of performing blending operations. **Veronique Bizet** is completing a manuscript on her work of a multiperiod MINLP model for catalyst deactivation. **Gabriela Garcia** has completed the incorporation of the new continuous time STN model by Christos as an interface

Steinar Hauan's Group

In his work on design algorithms for reactive separation processes, Warren Hoffmaster has complete his analysis of reachability in column sections and applied the results to columns with distributed feeds. Combined with optimal control studies, he can now predict the pareto optimal trade-off curve between the total amount of reactive holdup and the number of stages. Extensions to systems with highly non-ideal VLE and configurations with recycle streams and external reactors are in progress.

John Sirola (co-advised by Art Westerberg) is finishing up his studies of synthetic multi-objective optimization and is transitioning his agent system to engineering design. This fall, he has focused on two technical issues in agent-system design: (a) adaptive control of computational resources, and (b) effective management of shared memory resources. Recently he has started work on applying the agent system to the design of chip-based electrophoretic separation systems. Adesola Amosun has completed his classes and has started to study the flow of information in the agent system to prepare for AI-based control methods.

As part of a multi-disciplinary team, Anton Pfeiffer has completed a "DARPA Design Challenge" for microscale electrophoretic separation systems and demonstrated how one can fit multiple independent subsystems onto a single chip. Next he will seek to improve the subsystem layout by incorporating algorithms from computational geometry and also expand his optimization framework to include a less restrictive set of geometric shapes. Xiang He has demonstrated "proof of concept" for how one can approximate the performance of microreactors with incomplete mixing by a network of PFRs with crosstalk. The key challenge ahead is to identify the parameters needed to predict the network configuration without performing finite element studies.

Mike Bartkovsky (experimental focus) and Jane Valentine (modeling focus) continue their work on MEMS-based biosensors. Mike has completed a set of surface binding chemistry experiments using a quartz crystal microbalance apparatus and also started to study the vibration of our MEMS membrane using an (optical) microvision system. Jane has completed an initial study on sensitivity in multi-analyte systems and have started to look at how one should chemically functionalize the surface of the sensor to maximize robustness to incomplete adsorption.

Murni Ahmad has implemented independent routines for predicting the liquid-liquid phase behavior of protein-water-polymer systems and also for how target proteins partition between the different phases. The next challenge is to efficiently integrate the two, i.e. simultaneously converge the highly non-linear and poorly scaled set of equations to enable flowsheet design.

John Sirola has also implemented the first version of a new generation management software for distributed computing. The Remote Process Interface libraries allows rapid and fault-tolerant execution of processes in a Beowulf-style cluster. A paper is attached; the source code is freely available (CPL license) by email to hauan@cmu.edu.

Congratulations

Anton has successfully completed his Ph.D. proposal exam in November; Jane passed the Ph.D. qualifier exam in September.

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 PhD students, we now have a general strategy for very efficient NLP algorithms including rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. One resulting package, rSQP++, written in C++, has been adopted by Sandia National Labs as their framework for large-scale PDE-based optimization problems. Moreover, rSQP++ allows us to develop much more flexible NLP strategies that deal with structured Hessians, better exploitation of sparsity and changing active sets. Finally, the resulting strategy fits well with the object oriented construction of the program and also serves as a nice complement to the barrier strategies discussed below. In fact, our goal is to identify problems where different problem classes can exploit various SQP options. Most recently, we are interested in knowing when barrier approaches (see below) are favored over active set strategies. Carl Laird is currently working on extensions to rSQP++ for PDE-constrained optimization. In particular, he has augmented rSQP++ features to include the filter line search from Andreas Waechter along with a barrier method for NLPs (see description of IPOPT below). Combining this barrier approach with the flexibility of rSQP++ allows us to address much larger optimization problems while taking advantage of particular forms of matrix decomposition (e.g., dense, banded, sparse, iterative) and also exploit advanced computing architectures, particularly parallelism. In the future, this activity will allow us to address multiperiod problems for design under uncertainty as well as large-scale dynamic optimization problems within rSQP++.

In addition to modifying rSQP++, Carl Laird has developed 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. A paper that discusses this problem is listed below.

Barrier (Interior Point) Methods for Nonlinear Programming

Researchers: Maame Poku (Ph.D. started Fall, 2000)
Carl Laird (Ph.D. started Fall, 2001)

This project considers an efficient strategy for solving nonlinear programs using interior point (IP) methods, developed by Andreas Waechter, currently at IBM Watson. The resulting approach works either in the full space or can take advantage of the particular reduced space decomposition strategies that we have developed in previous work. The advantage of this approach is that it solves the nonlinear problem directly without first exploring the solution of the QP subproblem. In this way we avoid the overhead in solving highly constrained QPs, as these have the same level of combinatorial complexity as the original NLP problem.

Andreas developed and tested a number of variations to this approach that include the use of line search approaches, decoupling the barrier terms from the reduced Hessian approximation and options for both primal and primal-dual barrier terms. Along these lines, Andreas has discovered that Newton-based IP methods that are applied directly to NLPs can experience convergence failures. These failures are analogous to infeasible QPs that can be encountered in SQP but are much more subtle because the cause cannot be detected easily. In particular, Andreas has developed a counter-example that illustrates this problem, and has also developed a thorough analysis of this difficulty. In addition, Andreas has developed an improved line search algorithm that is based on a recently developed *filter* approach. This approach overcomes this convergence difficulty and Andreas has completed a rigorous convergence analysis of his approach. Numerical testing on thousands of test problems has also shown some significant performance improvements over other barrier algorithms. Major features of this approach are:

- an implementation that allows either full space or reduced space options for the barrier NLP. In particular, the reduced space option has been tailored to the structure of DAEs solved with collocation on finite elements.
- a filter line search approach that replaces the classical merit function for line searches
- a preconditioned conjugate solver for the null space step that replaces quasi-Newton updating and uses true second order information instead of just quasi-Newton information.
- an open source license has been prepared for this code. The current version of this code can be downloaded from: <http://www.coin-or.org>.

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 is used in blending applications and in the solution of MPEC problems. Here, Maame Poku has 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; a manuscript that compares these methods is listed below.

A number of improvements have recently been made by Andreas to this code. These include a more robust restoration step as well as iterative refinement in the solution of linear systems. Future plans for IPOPT include a recoding of the code into C. This will make the optimization methods much more portable for a variety of architectures.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: Arvind Raghunathan (Ph.D. started Fall, 1999)
Prof. Ricardo Perez (Pontifical University of Chile)
Dr. Soledad Diaz (Fulbright Fellow from PLAPIQUI, March-June, 2003)

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 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. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies. Arvind has also dealt with modeling a number of two level optimization problems that arise in engineering applications.

More recently, two important tasks under consideration are:

- Optimization of dynamic systems relating to models of cryogenic distillation processes. Here, Dr. Soledad Diaz is collaborating with Arvind to extend the MPEC problem to changes in phase behavior during startup and transient behavior. This approach was applied to both index 1 and (reformulated) index 2 systems and demonstrates for the first time how complementarity problems can be applied to dynamic processes. A manuscript that describes this approach and dynamic distillation results is listed below.
- Parameter estimation of a metabolic reaction pathway in *Saccharomyces Cerevisiae*. Working with Prof. Ricardo Perez at the Pontifical University of Chile, a metabolic model was formulated as a linear program. Its KKT conditions were then embedded within a nonlinear parameter estimation problem to form an MPEC, which was solved directly by IPOPT-C. The results showed an efficient and extremely effective way to elucidate the behavior of metabolic networks. A reprint that describes this work is listed below.
- Arvind has developed rigorous conditions for the global and local quadratic convergence of the IPOPT-C algorithm to solve MPECs. These results also provide a detailed guide to designing barrier algorithms for MPECs and a thorough comparison of related methods. Moreover, a detailed numerical comparison verifies the desirable features of this method.

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. Results on the optimization of these systems will be described in the next newsletter.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Researchers: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
 Shivakumar Kameswaran (Ph. D. started Fall, 2001)
 Yi-dong Lang (Jiansu Research Institute, Nanjing, China)

This project deals with simultaneous solution and optimization strategies for large-scale, dynamic optimization problems. 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. This is due to the possible presence of unstable modes in the forward direction. 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. 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. This approach easily allows for the addition of moving finite elements as well. A number of research topics have recently been addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization. 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.

Second, we are interfacing and benchmarking our algorithms to other popular modeling environments. In collaboration with Prof. Tsatsaronis at the Technical University of Berlin, Tobias Jockenhoevel incorporated the IPOPT algorithm within **OCC** (see <http://www.optcontrolcentre.com>), a MATLAB-based package for on-line optimization, system identification, off-line steady state and dynamic optimization and process monitoring. In particular, this package incorporates a number of discretization strategies (Gauss and Radau collocation, implicit Euler and BDF formulas) as well as the full algorithmic, graphical and modeling capabilities of MATLAB. With this collaboration we are exploiting the benefits of a MATLAB interface for dynamic optimization. This approach was applied to the dynamic optimization of the Tennessee Eastman challenge problem. A reprint that describes this work in detail and demonstrates extremely fast performance is listed below.

Our future work will be to combine these efforts. Here, inefficient features of third party software (e.g., MAPLE for generating derivatives) need to be replaced. Moreover, updates to IPOPT need to be transferred over to DynoPC and reduced space optimization strategies. Over the next year, our intention is to adopt the MATLAB framework and to couple it with the AMPL modeling language. Domain specific prototypes have already been developed (see next project) 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.

Over the past few months, Shiva Kameswaran 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. A manuscript that discusses these results will appear with the next newsletter. Moreover, these results points to the solution of singular control problems and problems with high index constraints. Both of 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.

Dynamic Optimization for Aircraft Conflict Resolution

Researchers: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
 Arvind Raghunathan (Ph.D. started Fall, 1999)

Through D. Subramanian and T. Samad at Honeywell, Inc. Arvind Raghunathan been pursuing an important research problem in aeronautics over the past two years. 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.

Development on these models has proceeded in a number of ways. First, we extended the 2-D models of Vipin Gopal to 3-D. As a result protection zones are now modeled as cylinders around each aircraft. Second, we applied a simple convex formulation of Sastry et al. to determine a good initialization for the NLP. This leads to much faster and more reliable performance of the conflict resolution problem. Finally, this approach was incorporated into a flight demonstration package called CROMA (Conflict Resolution of Multiple Aircraft), which combines IPOPT and AMPL within a MATLAB interface. As a result large problems with up to 8 aircraft and 4 obstacles have been solved efficiently.

Our current work is to extend these off-line CROMA 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 from the Iberoamericana University recently passed his qualifier and is working in this area. Currently, we have 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. A manuscript related to this approach is listed below.

Large-Scale Optimization for Fuel Cell Models

Researchers: **Cong Xu (PhD student started Fall, 2000, joint with Prof. M. S. Jhon)**
 Peter Follmann (exchange student from RWTH-Aachen)

Cong Xu is 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. A manuscript that describes this work is listed below. 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.

Future 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.

Optimization and Control of Pressure Swing Adsorption Systems

Student: **Ling Jiang (Ph.D. started Fall, 1999)**
 Yoshi Kawajiri (PhD started Fall, 2003)
 Seth Knaebel (MS started Fall, 2002)

Visiting Researchers: **Vanesa de la Torre (PLAPIQUI)**
 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. 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. *Preliminary 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.

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 are also currently being extended to separations of H₂ and CH₄ by Seth Knaebel, who has recently joined the group. He is modifying these models with new isotherm data. His work will also lead to the evaluation and optimization of a number of new PSA cycles.
- Ling has been extending this approach for separations of hydrogen and CO from refinery gases. These HyCO processes have a number of complications including multibed behavior, very tight purity specifications and challenging high dimensional dynamic behavior. A key feature of these systems is that they involve larger and more challenging multi-bed formulations. A manuscript that applies these multibed

strategies to the HyCO process is listed below. Currently, she is upgrading her optimization, sensitivity and DAE solvers to deal with parallel processing for multibed systems.

- Vanesa de la Torre recently joined the group and is developing 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.

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. In particular, Nikhil investigated more general classes of M-estimators for gross error detection within a simultaneous optimization framework. In particular, Nikhil has applied these approaches to an industrial project on carbothermic processes for silicon metal refining and casting. For these processes, dynamic furnace models are being developed (with Martin Ruszkowski and Prof. Erik Ydstie) and efficient strategies are needed for data reconciliation and parameter estimation for the existing process.

Nikhil has 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.

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. A manuscript that describes these results 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-July 03]
Research collaborator: Aldo Vecchietti
New Developments: Theoretical derivation of cutting plane method
New global optimization method for logic-based OA method
Addition of symbolic constraints in LOGMIP

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. One objective in Nick's work is to investigate whether one can theoretically determine whether the convex hull relaxation is strictly tighter than the big-M reformulation. A second objective is to develop effective solution methods of GDP problems, particularly for problems that may exhibit poor relaxations.

The first step in Nick's work has been to investigate how to project the higher dimensional equations of the convex hull into the original space of discrete and continuous variables. The basic idea relies on analytically solving for the parametric Lagrangean from the min-max feasibility problem applied to the convex hull constraints. While theoretically this approach provides a framework for the unambiguous comparison of the convex hull and big-M relaxation, it is very difficult to implement for large-scale problems. Therefore, there is motivation for developing a solution approach that relies on cutting planes, and can generally be embedded within a branch and cut algorithm. The major steps of the algorithm are as follows. We 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, where one might continue the derivation of the cutting planes at each node.

Nick has developed a solid theoretical derivation of the cutting planes for the 1, 2 and infinity norms. The basic framework for the derivation relies on the use of subgradient optimization, since the value function for the 1 and infinity norm are nondifferentiable. It is only the 2 norm that is differentiable. The useful aspect of this derivation has been to realize that the selection of the best norm is problem specific, since theoretically one cannot prove the superiority of one norm over the other.

Nick has applied his cutting plane technique to a 5-process retrofit problem that Jennifer Jackson formulated as a GDP problem for her Ph.D. work. In that problem the convex hull formulation requires 9 nodes and has only a gap of 0.25%, whereas the big-M MILP requires 660 nodes and has a gap of 19.5%. Using the cutting plane technique with infinity norm the gap is reduced to 13.5% with one cut, and to 0.36% with 10 cuts. The number of nodes required in each case were 458 and 47, respectively, thus showing the potential of the proposed method. Nick has also applied his technique to a strip-packing problem that consists of finding the shortest length of a rectangle with fixed width that can accommodate a given set of rectangles with fixed dimensions. This problem can be formulated as a GDP problem. Nick has formulated this problem with big-M constraints, convex hull reformulation and also solved it with the cutting plane method. Using CPLEX 7.5 the solution of a 10 rectangle problem required 1,782,291 nodes and 323 secs, while the convex hull required 45,195 nodes and 60.25 secs. Adding 1-norm cut in the root node reduced the number of nodes for the big-M model to 714,007 nodes and the total time to 126.7 secs (including separation problem). Adding 5 cuts reduced the number of nodes to 51,007, and the time to 7.6 secs, about one tenth of the full space convex hull model. It should be noted that Nick received the first prize at the CHEGSA Symposium for the presentation of this work.

Nick is also investigating the relationship of our proposed cutting planes with other cuts such as Gomory and mixed-integer rounding cuts. Although our cuts do not exhibit the closure property (i.e. in the limiting case they do not converge to the integer convex hull), preliminary proofs have shown that our initial cutting planes that we generate are stronger. Nick is also studying the lift and project method in order to provide a rigorous derivation for the cutting planes.

Lorena Bergamini

Lorena, a Ph.D. student from Argentina who was this first semester with us, has been developing a new deterministic algorithm for the global optimization of process networks that are formulated as Generalized Disjunctive Programs and that involve nonconvexities, which may lead to suboptimal solutions. The global optimization algorithm does not require spatial branch and bound searches and 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 considering 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 has assumed that the functions involved are sum of convex, bilinear, and concave terms. The logic-based OA algorithm consists of an iterative procedure in which the problem is decomposed into continuous and discrete optimization subproblems. The continuous optimization subproblem requires the solution of reduced NLP subproblems, which are obtained by fixing the Boolean variables, while the discrete optimization is obtained through the solution of MILP master problems. In order to rigorously maintain the bounding properties of the MILP master problem for nonconvex problems, 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. It should be noted that binary variables are needed for the discrete choice of the corresponding subdomains. Linear fractional functions are treated in a similar way. Piecewise linear subestimations replace the concave terms.

Application of the logic based OA algorithm for nonconvex GDP also requires the solution of the NLP subproblems to global optimality, which can be performed by fixing the topology variables in the MILP and by successively refining the grid of the approximations. Alternatively, any general purpose NLP algorithm for global optimization (e.g. BARON code) can be used. It should be noted that the NLP subproblems are reduced problems, involving only continuous variables related to a process with fixed structure. This allows the tightening of the variable bounds, and therefore reducing the computational cost of solving it to global optimality. Lorena has developed a variable bound reduction for this purpose. Initial NLP subproblems also have to be solved in order to obtain feasible points to derive linearization of the convex terms. If there are no convex terms the algorithm starts with the first master problem, derived using the bounds to construct the approximation functions for bilinear, linear fractional and concave terms. 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. Another example dealt with the synthesis of water treatment systems that incorporate liquid membrane separation units in which the algorithm required 14 minutes to find the global optimum.

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 that he 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 (eg $g(x) \leq 0 \Rightarrow f(x) \leq 0$) can be systematically converted in the form of disjunctions. The intent is also to be able to accommodate MINLP models in algebraic form, as well as hybrid models that are partly expressed as disjunctions and partly as equations.

In the current version of LOGMIP the code 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 small and medium sized problems that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. Aldo has also automated the logic-based OA algorithm, which is suitable for nonlinear GDP process network problems. An example of part of the input in GAMS that can be accomplished with LOGMIP is shown below:

```
DISJUNCTION D1,D2;  
D1 IS  
IF Y('1') THEN
```

```

EQUAT1;
EQUAT2;
ELSIF Y(2') THEN
EQUAT3;
EQUAT4;
ENDIF;

D2 IS
IF Y(3') THEN
EQUAT5;
ELSE
EQUAT6;
ENDIF;

```

As for the more impressive numerical results with LOGMIP, in one of Jennifer's models, Aldo found that the big-M formulation of her retrofit planning problem takes about 1745 nodes with OSL, while convex formulation through LOGMIP only requires only 9 branch and bound nodes!

Over the last few months Aldo has completed in LOGMIP the definition of disjunctions over sets and subsets with the conditional statement operator WITH. An example, which previously required specifying the disjunction for each subset, is given below where it can be seen that only one statement is required for defining the disjunction:

```

SETS I jobs / A, B, C, D, E, F, G / ;
ALIAS (I,K) ;
SET J stages / 1*5 / ;
ALIAS (J,M) ;

SET L(I,K,J) /A.B.3, A.B.5, A.C.1, A.D.3, A.E.3, A.E.5, A.F.1, A.F.3, A.G.5,
B.C.2, B.D.2, B.D.3, B.E.2, B.E.3, B.E.5, B.F.3, B.G.2, B.G.5,

C.D.2, C.D.4, C.E.2, C.F.1, C.F.4, C.G.2, C.G.4,
D.E.2, D.E.3, D.F.3, D.F.4, D.G.2, D.G.4,
E.F.3, E.G.2, E.G.5,
F.G.4 / ;

DISJUNCTION D1 (I,K,J) ;
D1 (I,K,J)
with (L(I,K,J)) IS
IF Y(I,K,J) THEN
NOCLASH1 (I,K,J) ;
ELSE
NOCLASH2 (I,K,J) ;
ENDIF;

```

As for the propositional logic, Aldo is implementing the special constructs ATLEAST, ATMOST, EXACTLY to specify that the sum over of subset of variables with a given cardinality, the most common choice being one. Also, the plan is for LOGMIP to accept logic propositions in symbolic form without the need of translating them into linear inequalities.

We should also remind that LOGMIP has implemented the logic-based outer approximation method developed by Metin Turkey for nonlinear problems. An extensive website on LOGMIP is now also available, <http://www.ceride.gov.ar/logmip/>

Modeling and Optimization of Hybrid Systems for Supply Chain Problems

New developments: *Application to State-Task Network*

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

The objective of Ashish's project is to develop a new hybrid systems framework for modeling supply chain networks. The basic idea in Ashish's project is 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. In terms of the optimization of a supply-demand network, the problem can be viewed as finding the trajectory which maximizes profit by enabling multiple transitions during a range of times; the free variables are which state to transition to and when to transition. Two major classes of problems can be considered. Optimization over a finite horizon for which initial conditions are specified, and infinite horizon, for which one can either apply a cyclic policy, or else a model predictive control approach.

For both cases Ashish has 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 is also applying his modeling framework to the classical State-Task Network example by Emilia Kondili. An interesting question will be to see whether the discrete time formulation can be readily obtained as a particular case of the continuous time model.

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: *Decomposition technique for optimizing complex columns with tray-by-tray
Synthesis of thermally integrated distillation columns with short-cut models*

Students: **Mariana Barttfeld (Ph.D. INGAR)**

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

This project has dealt 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 is to develop rigorous optimization procedures that can make use of tray by tray models. Mariana Barttfeld from Argentina is concentrating 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 successfully defended her Ph.D. degree in Argentina, having 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. Mariana coupled the MINLP and GDP models with an NLP thermodynamic initialization model that assumes that all the potential trays are present at the final solution. For the MINLP model, a reduction of candidate trays was performed to decrease the number of trays. From several ternary mixtures that she considered the most effective MINLP model proved to be case of variable feed and reboil location. For the GDP the case of fixed reflux, feed and reboiler trays, and all other as conditional trays, proved to be the best,

which in fact is the representation that was used by Hector Yeomans. For the MINLP case convergence was only achieved with the initialization procedure. For the GDP case it helped, but it was less critical. 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.

Mariana also investigated the synthesis of superstructures for complex column configurations (e.g. Petlyuk, 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 has 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.

Jose Caballero

Jose has been addressing 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. Agrawal (2000) has addressed this problem and proposed a procedure to draw by "hand" the thermodynamically equivalent structures. 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 applied the logic constraints to simplified MILP problems involving mixtures of 4 and 5 components. Jose is currently developing nonlinear GDP models based on STN superstructures for synthesizing thermally integrated columns using short-cut models.

In the last few months 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 it 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.

Synthesis of Crystallization Processes

New developments: *Initial MINLP optimization of crystallizer configurations*

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 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, has proved to be rather challenging due to the nonlinearities involved. To circumvent this problem Carlos has developed a two-stage procedure to increase the robustness of the convergence. It should also be pointed out that the proposed model matches fairly well real plant data. The proposed model is being used to optimize the topology of the flowsheet and as well as the operating conditions. The first step has 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 preliminary results, which have been obtained through an MINLP model, has predicted structure with fewer crystallizers than the ones used in practice. In order to perform the more extensive superstructure optimization, we intend to explore the use of LOGMIP with the logic-based outer-approximation scheme.

Multistage Stochastic Optimization for Design and Planning of Oilfield Infrastructures

New Developments: *Generalization of variable scenario tree for multistage stochastic optimization and application to process planning problem*

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

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 has developed a multistage stochastic optimization in which the investment decisions define the structure of the scenario tree. This type of problem, which has almost not been reported in the literature, Vikas has been generalizing for general purpose linear multistage stochastic programming.

Vikas discovered a very subtle point that is rarely covered in the stochastic optimization literature. The specific point in the gasfield problem is that the size and deliverability are "endogenous" parameters rather than "exogeneous" (e.g. prices), which means that the scenario trees depends of the time when the decisions are made. As an example, if the uncertainty is price, we can have low (L) and high (H), and we have 2 periods, then there are a total of 6 scenarios in the tree: period 1 (H or L), period 2 (HH, HL, LH, LL). On the other hand if the uncertainty is size, then if the platform is installed in period 1, the scenarios are period 1 (H or L), and also period 2, since once the platform is installed the uncertainty is resolved. If on the other hand the platform is installed in period 2 then in period 1 there is only one scenario (i.e. H or L is irrelevant), while in period 2 there are 2 scenarios (H or L). 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 developed an approximate solution technique for the gasfield problem 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. 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 uses 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. Vikas has shown that this method converges to the rigorous optimum for the case of one uncertain field. Vikas has applied this method to 4 problems. The largest one involved 4 certain and 2 uncertain fields in 8 years. The number of scenarios is 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, which incidentally can be reduced to about one hour with trivial parallelization. This solution, which had an expected NPV of \$79 million, had a \$5.6 million improvement over a deterministic solution.

Given the success of Vikas' work in the multistage stochastic optimization of gasfield problem, he considered a manufacturing problem that has been addressed by Jonsbraten. The problem is similar to a lot-sizing problem but also involves manufacturing parts in different sizes. The large ones can be cut to smaller sizes to adjust for the changes in the uncertainties in the demand. There are also uncertainties in the cost of producing the parts, which is an endogenous uncertainty. What Jonsbraten did was to propose a branch and bound method in order to handle the problem that the scenario tree is a function of the decisions (i.e. what sizes to produce at each time period). 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 endogenous uncertainties are not revealed because no sizing decisions are made. Otherwise, they "explode" into the nodes that define the events in the tree. While the closed form model is conceptually is very 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 reduces 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 is developing 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 nearly completed the implementation of this algorithm for which preliminary results have proved to be very encouraging. Also, in order to illustrate the application of this approach to a process related problem, Vikas has considered the problem in which 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. The specific problem involves one uncertainty in the product demand, and two uncertainties in the yields. By using a deterministic approach the solution that is obtained by accounting for recourse is an expected cost of \$422,868. In contrast the proposed solution yields an expected cost of \$409,222. Both solutions differ in the selection of unit for expansion as well as its timing. The big-M reformulation of the full-space problem involved 240 binary variables and 3,531 constraints, while the formulation with only the adjacent pairs has 2,601 constraint and same number of 0-1 variables, yielding a 50% reduction in the CPU time.

Scheduling of Batch and Continuous Multiproduct Plants

***New Development:** Application of STN MILP/CP hybrid method to multistage and single stage problems*

Student: Christos Maravelias (Ph.D. started January 2000)

Christos Maravelias has been working in developing a new continuous-time MILP model for the State-Task-Network (STN) representation for batch scheduling. Given the computational difficulty in solving this problem he has also developed a hybrid solution method that integrates CP (Constraint Programming) and MILP. Finally, Christos has also shown how the discrete time STN model can be used for minimizing the makespan.

Christos has developed a new continuous-time MILP model for the short term scheduling of multipurpose batch plants. The new model relies on the State Task Network (STN) by Kondili, Pantelides and Sargent (1993) and accounts for resource constraints (other than units), variable batch sizes and processing times, various storage policies (UIS/FIS/NIS/ZW), and accounts for changeover times. Christos has treated the time domain through intervals of unknown duration, and in which the continuous events that define the start times of the operations are matched with the start times of the intervals. Christo's model is more general than previous works, which may either overconstrain the problem, or else produce infeasible solutions as is in fact the case in the Ierapetritou and Fludas (1998) model that is based on time events. The idea of decoupling tasks and units is used in the representation of Christos' model. He formulated this model first as a hybrid GDP/MILP model, and then reformulated it as an MILP model in which a novel way of expressing assignment and time matching constraints leads to formulations with fewer binary variables. The interesting feature of the model is that it can be solved for profit maximization, cost minimization for fixed demand, and for makespan minimization. The largest problem involved 10 tasks and 14 states in 12 time periods with resource constraints in cooling water, and low and high pressure steam. The model had as objective to maximize profit, and involved 180 binary variables, 1587 continuous variables and 3067 constraints.

CPLEX solved this problem in 2,107 nodes and 63 secs. Christos also has extended the model so as to handle due dates.

Christos has also developed a hybrid integration of MILP and Constraint Programming (CP) in solving the new continuous STN model. As opposed to the case of Vipul Jain where the MILP and CP partitioned in a direct way between assignment and sequencing for batch scheduling, in this case the partition is less obvious. The basic idea consists in reformulating the determination of tasks in the STN with an aggregated MILP model that provides a valid bound and determines the number of times each task is performed. This is then followed with a CP problem, which for the fixed tasks determines the assignment of equipment and the timing of the operations. The sequence of iterations is continued by adding special integer cuts until the bounds converge. There are three types of integer cuts: (a) to eliminate previous solution, (b) to eliminate infeasible assignments in subnetworks, (c) to eliminate multiple equivalent solutions for the case of identical parallel equipment. The MILP formulation is also tightened through preprocessing by reducing the range of release and completion times of the batches. Christos has successfully solved several problems with the various objective functions using CPLEX for the MILP and ILOG-Scheduler for the CP part. For problems involving profit maximization reductions of one or two orders of magnitude were achieved. For the case of makespan minimization the reductions were even more dramatic. For example a STN problem with 19 tasks, 27 states and 8 equipment, the MILP problem could not be solved after 10 hours of CPU time, while the hybrid model only required 5 secs and 9 major iterations! Christos has completed the manuscript on this work which has been submitted for publication.

The most recent development has been to apply the hybrid MILP/CP method to special cases, including multistage plants and single stage with parallel units. The latter in fact corresponds to the problem that Vipul considered in his Ph.D. thesis for which he demonstrated order of magnitude reduction compared only to MILP or only CP methods. Christos was able to obtain reductions of up to a factor of 10 compared to the results by Vipul, demonstrating the generality of his integrated MILP/CP approach.

Optimal Scheduling of Refinery Operations

New development: *New multiperiod MILP model*
Postdoctoral fellow: **Carlos Mendez (started Jan 2003)**

Carlos been working 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 is 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 has developed a novel MILP model for blending that is based on the idea of computing the mismatch in the nonlinear properties from which a correction factor is inferred for the MILP model. This model has been tested with several gasoline mixtures and yielded approximations that are very close to the nonlinear model. The advantage of the proposed blending model is that it can be incorporated readily as part of a multiperiod MILP model for optimizing the scheduling problem that involves decisions on blender and tank allocation, as well as their timing. Furthermore, Carlos has also developed a continuous time model that makes use of time slots. For problems involving 10 days of operation, 3 blend headers, 12 storage tanks, 3 final products, 9 product requirements and 5 product due dates has shown to produce not only significantly higher profit solutions, but also reduced computational costs. One of the next steps that Carlos is starting to investigate is the use of pipelines to eliminate the finished product tanks.

Uncertainty in the Scheduling of Batch Processes

New development: *Shrinking horizon strategy for multi-stage programming for demand uncertainty*
Student: **Jayanth Balasubramanian [Ph.D. started November 1998]**

Jayanth, who successfully defended his Ph.D. thesis in April, investigated batch scheduling problems in which the uncertainties considered are processing times and demands. In the former case the problem is to find a schedule that

minimizes the expected completion time, while in the latter the objective is to maximize the expected net present value.

Jayanth focused his initial work on flowshop and parallel line scheduling problems, as well as scheduling for new product development. In these cases the major source of uncertainty considered was the duration times. Jayanth developed a branch and bound procedure for flowshops with zero wait policy in which the key idea was to use for a fixed sequence the analytical expression proposed by Karimi to calculate the expected completion time. The second important property is that when the tasks in the flowshop are replaced by the expected process times, the completion times yield a *lower bound* to the expected completion time. Third, Jayanth devised a clever branch and bound enumeration in which he sequentially “explodes” the full probability space on products that have been fixed in the sequence. The products that have not been fixed are replaced by expected values, which guarantees the lower bound properties. In the implementation that Jayanth developed in Java he was able to solve problems with up to 9 products and 3 stages with 7×10^{12} scenarios. Jayanth also extended the method for flowshops with UIS policy and for continuous distribution functions using discretization schemes that rely on the fact that for univariate functions exact discrete approximations are possible for higher moments by the appropriate selection of discrete points that correspond to roots of polynomials for Gaussian integration.

Motivated by the need to develop computationally efficient methods for optimizing schedules with uncertain tasks, Jayanth next developed a non-probabilistic approach that relies on the use of fuzzy sets. In terms of completion times, this is almost equivalent to interval arithmetic where the major result that one can obtain are lower and upper bounds for the completion time for a fixed schedule. Using triangular fuzzy numbers, the equivalent to the expected completion time reduces to the average completion time integrated over all parametric intervals that are centered to the center point, and with deviations proportional to the bounds of the completion time. To extend this approach to optimization one can formulate a corresponding MILP model, which Jayanth did for flowshop plants (single units per stage and parallel units), and for the new product development problem. In the case of flowshops with 8 products and 4 stages, Jayanth's procedure required about 28 sec while the probabilistic approach required 4 hours! Jayanth also developed a reactive tabu search procedure for solving much larger problems. Jayanth also solved new product development problem with 65 tests. The resulting MILP involved 4061 binaries, 8794 continuous variables and 267,912 constraints, and was solved in about 45 minutes with CPLEX.

In the last part of his Ph.D. thesis Jayanth addressed the optimization of the short-term scheduling of a multi-product batch plant, while taking into account the uncertainties in the demands for the products. Given are N products that can be manufactured in a batch plant in L modes (characterized by a specific batch size and product-dependent processing time). The demands for these products are described by discrete probability distributions; and these demands are to be satisfied at the end of the scheduling horizon. The costs involved are those for (i) holding inventory over the horizon, (ii) excess inventory at the end of the horizon, (iii) lost demand (due to inadequate production); while the revenues are from selling the products. The problem then is to obtain a schedule that maximizes the expected profit, where the schedule consists of deciding the allocation of the equipment to the appropriate mode of production of a product over the time horizon. Unlike previous work, Jayanth has assumed that some of the demand can actually be unsatisfied, due to limited production capacity. Thus, the problem also consists in choosing the optimal amounts to be produced for each product. Jayanth showed that it is possible to improve on the conventional two-stage scheduling approach in which a fixed schedule is selected for all scenarios. Jayanth formulated a multi-stage stochastic MILP by considering that the time horizon is subdivided into several subperiods at the end of which rescheduling is performed. To solve this problem Jayanth developed a shrinking horizon strategy somewhat similar to the one that was used by Vikas in his work. The strategy is based on solving successively two-stage programming stochastic MILPs in which decisions over the subperiods are successively fixed. In this way, one starts optimizing over the entire horizon. After the solution to this problem decisions are fixed in the first subperiod and the horizon is “shrunk” by excluding the first subperiod. For the next stage one considers the various outcomes of the discrete probabilities in the first subperiod, and each of them is solved as a two-stage problem for the remaining horizon. The procedure is repeated until only one subperiod is left. It should be noted that the result then provides not a single schedule, but rather a sequence of schedules that can be adopted depending on the realization of events at each subperiod. Examples include single unit processing plants and large State-Task Networks. Among the larger problems Jayanth solved an 8-task, 6-unit, 4-product STNs with three possible processing modes for each task over a 18-unit time horizon. The deterministic model for this problem had 456 binaries, and 4000 constraints. The multistage stochastic formulation for this problem had 1104 binaries and almost 23000 equations and could not be solved to even within 10% of optimality in 10 CPU hours. With the shrinking horizon strategy of successively

solving two-stage stochastic MILPs, Jayanth obtained solutions that improve the expected profit by 18% over solving the deterministic model once, and 6.5% over solving successive deterministic models, in very reasonable CPU time (~10-20 minutes).

Integration of Product Testing and Planning of Batch Manufacturing Facilities

New Developments: *Formulation and solution method for investment of resources for testing*

Student: **Christos Maravelias (Ph.D. started January 2000)**

This research project has also been part of Christos' work and deals with the development of an optimization model and solution method for the simultaneous testing for new product development and planning and design of batch plants. The specific problem, which arises in agricultural chemicals and pharmaceuticals is one where a time horizon is considered over which a set of new products that have been discovered in research are to be tested for certification to meet FDA regulations. Costs, duration and probabilities of success of each test are known. Given also are existing batch manufacturing facilities, as well as potential plant configurations that may be used to manufacture the potential products. During that time horizon it is also possible that existing products may be withdrawn from manufacturing. The problem consists in determining the schedule for testing of the products, as well as the selection of batch manufacturing facilities (existing or new) for their manufacturing in the event that the products pass all the tests. The objective is to maximize the expected net present value of the project. In order to account for uncertain outcomes, multiple scenarios must be considered in terms of possible successes and failures of the tests for the new products.

Christos developed a large-scale MILP model for this problem. The proposed model includes scenarios that may arise depending on the outcome of the tests for the products. In order to effectively solve the resulting MILP model, Christos has developed a Lagrangean decomposition scheme where the constraints that tie the testing and the manufacturing planning problem are relaxed by dualizing these constraints. The idea then consists of iterating between the dualized problem, which can be decomposed and provides an upper bound to the profit, and a feasible MILP problem that provides a lower bound. Although the gap cannot be guaranteed to be closed, computational experience has been encouraging. One of the examples considered by Christos involves a plant with 4 stages that manufactures 4 products. Two new products are considered in the pipeline, each requiring a total of 10 tests with some precedence constraints. This then also leads to four scenarios in the model. The MILP model involves 718 binary variables, 11,216 continuous variables and 11,173 constraints. With CPLEX it took 57 secs to solve this problem; with Lagrangean relaxation only 37 secs. In a larger example, the reduction was from 830 secs to 252 secs.

Since the major bottleneck in the above procedure is the part of the resource constrained MILP scheduling problem, Christos has revisited that problem, which Vipul Jain had addressed. Christos initially explored a number of alternative solution methods. At the end the most successful approach is one that combines logic cuts with a decomposition procedure. The logic cuts are based on implied precedences that can be derived from either fixed precedences, or precedences that arise in the selection of sequences. As an example, if A is followed by B, and B followed by C, then A followed by C is an implied precedence. Christos also applied these cuts in explicit form or as violated cuts in the root node. The former case required adding 239,000 constraints, while the latter required 18,000. Both, however, produced the same reduction of the LP relaxation (6,176 to 5,001) Although the implied precedences greatly improve the LP relaxation, larger problems are still expensive to solve. This motivated the idea of decomposing the problems by products. Those precedences that are activated (i.e. corresponding binaries take value of one) are fixed in the joint problem for all the products. This solution to the overall MILP provides a heuristic, which however, can be shown to have a tight bound. As an example, Christos considered a problem with 4 products with 60, 30, 40, 20 tests, respectively. The full space MILP has 14,000 0-1 variables, 3,300 continuous variables and 26,000 constraints. CPLEX required 6,900 secs to solve the problem with a 5% optimality gap, while the proposed method required 520 secs, finding a solution within 0.5% of the optimum. Christos is currently automating the proposed solution method in the new version CPLEX 8.0.

Christos has also considered a more general form of the resource-constrained problem for new product development. Previous models have assumed that the resources available for testing such as laboratories and scientists are constant throughout the testing horizon, and that all testing tasks have fixed cost, duration and resource requirements. In order to be able to handle more effectively a number of potential products in the R&D pipeline Christos has

considered in the model the option to install/hire additional resources. Also, the type and amount of resources can be chosen for some tests to reduce their duration. Christos has developed a new scheduling MILP model that addresses these issues to optimize the overall costs. More specifically, the model (a) allows for installation of new resources during the course of testing, and (b) handles cost and duration of tests as functions of the type and amount of the resources assigned to each test. To enhance the solution of the model Christos has considered some of the logic inference cuts as well as a reformulation with disaggregated variables and a procedure for the tightening of the big-M constraints. The solution of a single large-scale problem is also avoided with the heuristic decomposition that relies on solving a reduced mixed-integer program that embeds the optimal schedules obtained for the individual products. The proposed algorithm has been shown to be one to two orders of magnitude faster than the full space method, yielding solutions that are optimal or near optimal. In an example with 3 products, 28 tests and 6 existing testing units and 6 new potential ones, the proposed solution method required 180 secs with CPLEX, while the full space model could not be solved to optimality after 5 hours of CPU time, and only yielded a solution that was 40% less profitable than the one of the decomposition method. Christos has recently completed a manuscript on this problem.

Optimization Approaches for Metabolic Engineering

New developments: *Global optimization formulation for inverse problem*

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. However, using NMR data to best fit a linear combination of fluxes that minimizes a sum of squares deviation is problematic because a non-linear optimization problem can result that is highly non-convex due to the bi-linear and tri-linear terms that arise with the isotopomer distribution vectors. To circumvent the problem of getting trapped in local solutions, Soumitra has investigated 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 bacteria 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.

Optimal Multiperiod Planning for Catalyst Replacement

New developments: *Honorable mention for poster at AIChE Meeting*

Research Assistants: **Veronique Bizet (started September 2002)**

This project by Veronique Bizet is a joint collaboration with Atofina Chemicals (TOTAL) through Nikola Juhasz. The problem assumes that a continuous plant is given that produces a product with seasonal demands. The process involves a reactor that undergoes catalyst deactivation. Replacing the catalyst is a rather involved operation that requires significant amount of time, as well as careful coordination with the inventory management. Optimization variables in the process include the reactor temperature and the recycle rate, which to some extent can be

manipulated to compensate for the deactivation. Given a long term horizon (few years), the problem consists in determining the timing for the replacement of the catalyst, as well as the optimal operating conditions and inventories on a monthly basis.

Due to the complexity of the process, a semi-empirical model is used that provides reasonable fit with the plant data. This model is used as a basis for developing a multiperiod MINLP model for deciding the optimal catalysts replacement, and operating conditions. The model uses concepts of disjunctive programming and logic optimization that can readily handle constraints on temperature profiles. Through numerical experimentation Veronique discovered that while DICOPT often finds good solutions, the nonconvexities in the model can lead to suboptimal solutions. In order to try to identify the global optimum, Veronique has developed a partitioning strategy that relies on solving subproblems over subintervals that lead to smaller MINLP problems. For the case of more than 2 changeovers the alternatives are represented through a tree of subintervals which are then also optimized to find the best solution. Also, given the large-size of the MINLP model for long time horizons (4 to 8 years), Veronique has investigated the implementation of generalized Benders decomposition. Since not unexpectedly, the lower bound was found to be rather weak, she reformulated the MILP master problem by transferring most linear constraints of the MINLP into the master problem. The computational results have shown that the partitioning strategy leads to a more robust method that is more likely to yield the global optimum. As an example, Veronique solved a 108 period problem (9 years) with up to three catalysts. The corresponding MINLP involved 816 0-1 variables, 8,013 continuous variables and 33,230 constraints. DICOPT solved this problem in 351 secs, but obtained a suboptimal profit of 191.77. In contrast the partitioning procedure took 1880 secs and found a profit of 200.37. Generalized Benders also found this solution but required 3369 secs.

Veronique also received an honorable mention as the best poster from the CAST Division for the paper "Optimization Model for the Production and Scheduling of Catalyst Changeovers in a Process with Decaying Performance" by Bizet, V.M., N. Juhasz and I.E. Grossmann. She is presently writing up her work as a paper.

Software for MINLP Optimization in Design and Scheduling

New Developments: *Continuous time STN model*

Research Assistants: **Gabriela Garcia (started March 2000)**

Collaborators: **Dr. Zdravko Kravanja, Univ. Maribor, Slovenia**

As part of the web framework for accessing various interfaces, which is available in:

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

Gabriela has recently completed the implementation of the STN interface with the recent continuous time MILP model by Christos. The interface STN also implements the discrete time STN model.

Another recent interface is a GDP model by Mariana Bartfeld for distillation column design using tray-by-tray models. Other interfaces that Gabriela has implemented include BATCHSPC, BATCHMPC, CYCLE, DECA, MULTISTAGE, NETCHAIN, SYNHEAT, and WATER (see brief description below). She has recently added the programs EXTRACTOR (liquid-liquid extraction) and PRODEV (testing for new product development). The web access will make it easier to access these interfaces. Hopefully this will also promote greater use by the members of the CAPD. The idea in the framework developed by Gabriela is that the interfaces all have a "common look" as the current PC interfaces. This project was inspired by the joint collaboration with Dow in which the final implementation was performed on a web-intranet system. Regarding our collaboration with Zdravko Kravanja, he has continued developing the new code MIPSYN that is PC-based and that makes direct use of the recent developments in disjunctive programming for flowsheet synthesis.

The current list of programs that we have available or nearly completed can be examined in our website, <http://egon.cheme.cmu.edu>. The programs are as follows:

Synthesis:

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

Batch design:

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

Scheduling:

<i>PARALLEL</i>	MINLP continuous multiproduct scheduling on parallel lines Features feasibility preanalysis (<i>Sahinidis</i>)
<i>MULTISTAGE CYCLE</i>	MINLP continuous multiproduct in multistage plants (<i>Pinto</i>) LP/MILP aggregate flowshop scheduling (cycle time/makespan) Includes loop tracing algorithm (<i>Birewar</i>)
<i>STBS</i>	MILP short term multistage scheduling (<i>Pinto, Bolio</i>)
<i>CRUDEOIL</i>	MILP model for refinery scheduling (<i>Lee, Pinto</i>)
<i>DECAY</i>	MINLP model for scheduling of clean-up of parallel furnaces (<i>Jain</i>)
<i>UTILPLAN</i>	MILP multiperiod model for utility plants (<i>Iyer</i>)
<i>PRODEV</i>	MILP model for scheduling of tests in new product development (<i>Schmidt, Najimas</i>)

Planning:

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

Steinar Hauan's Group

Feasibility and Economics of Reactive Separation Systems

Student: Warren Hoffmaster (PhD, started Jan 2000)

BACKGROUND

Over the last decade, the idea of combining reaction and separation has shown a significant industrial potential. As of today, most major chemical companies are considering or implementing processes such as reactive distillation columns and membrane reactors along with more well known variants like absorption columns with chemical reaction, multiphase reactors and reactive heat exchangers.

Many claims have been made as to why these units sometimes perform better than conventional equipment; among them are improved reaction selectivity, higher energy efficiency and lower capital cost. However, the design and optimization of such multifunctional (or hybrid) units are still more of an art than science. When, for instance, trying to understand how a reactive distillation column really works, several different views are possible: Are they reactors in which separation occurs, distillation column with chemical reactions or are they neither and require a new set of theories? No matter the answer, there is still a substantial gap in our knowledge in systematically addressing the interactions between fundamentally occurring processes. Consequently, their effect on feasibility and economic potential is far from obvious.

Using the theory of generalized difference points developed in collaboration with Art Westerberg's group, we seek to answer the following two questions:

- 1) What is the product composition region -- i.e. all products reachable for a given feed -- for systems combining reaction and separation?
- 2) Given a set of feasible processes involving both sequential and simultaneous reaction and separation; where is the economic optimum as a function of system specification and process operation?

Our work has identified a decomposition strategy wherein a set of internal cascade sections may be analyzed individually. The goal is first to identify the reachable compositions in all possible section types and then develop an optimal control or MINLP formulation that would identify the best designs. A key point here would be that the feasibility of the NLP subproblems would be known a priori and combine these insights with optimal control of reaction holdup and systematic considerations of columns with distributed side feeds.

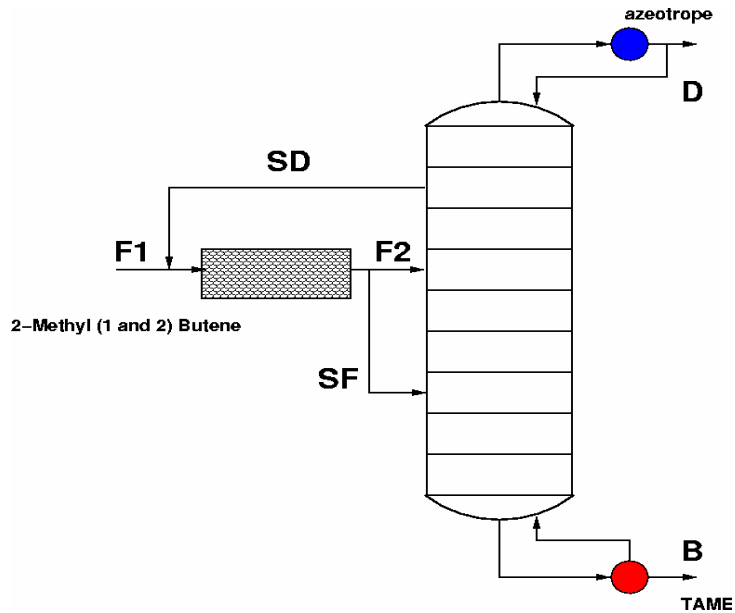
PROGRESS

Over the last few months, Warren has completed two case studies of reactive distillation systems: Olefin metathesis of 2-pentene and etherification for production of tert-amyl methyl ether (TAME). In addition to using traditional design variables like reflux ratio and the number of stages, he has also considered the amount of reactive holdup (and thus catalyst) required to obtain a desired set of products. He also has considered conceptual and optimization-based strategies for improving column design by using (a) distributed feeds, (b) subcooled and superheated feeds, (c) side feeds and side draws, (d) external reactors in front of and in parallel with the distillation system.

The first step has been to extend our method for identification of feasible production compositions for reactive separation systems to handle complex column, i.e. configurations with multiple input and output streams. The standard feasibility criterion for cascaded separation -- overlap of reachable end-products in composition space-- has been used to either rigorously demonstrate infeasibility or generate starting points for subsequent optimization. The results are being written up for publication, but some of the most interesting results include:

- an even distribution of reactive holdups is substantially worse than
- even with a single reactant ($2A \rightarrow B + C$), distribution of the external feed stream may reduce the total amount of catalyst required in a design; in particular if combined with feed qualities outside the normal range of zero to unity.
- feasible region analysis and computational methods are getting mature enough to handle more complex columns in a reasonable amount of time.

An example flowsheet is shown in the figure below



Agent Systems in Engineering Design and Optimization

Students: John Sirola (PhD, started Jan 2001) and Adesola Amosun (MSc, started Feb 2003)

BACKGROUND

Co-advised by Art Westerberg, John is studying how to pose and solve very large design and operation 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

His approach assumes that computing capabilities will increase many fold this next decade and that the computing resources will be available in the form of distributed computer cluster. This work continues that started by Ken Tyrer on the synthesis of flexible separation processes.

John is studying the use of agent-based systems. In these systems many agents 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?

Our strategy has three algorithmic levels:

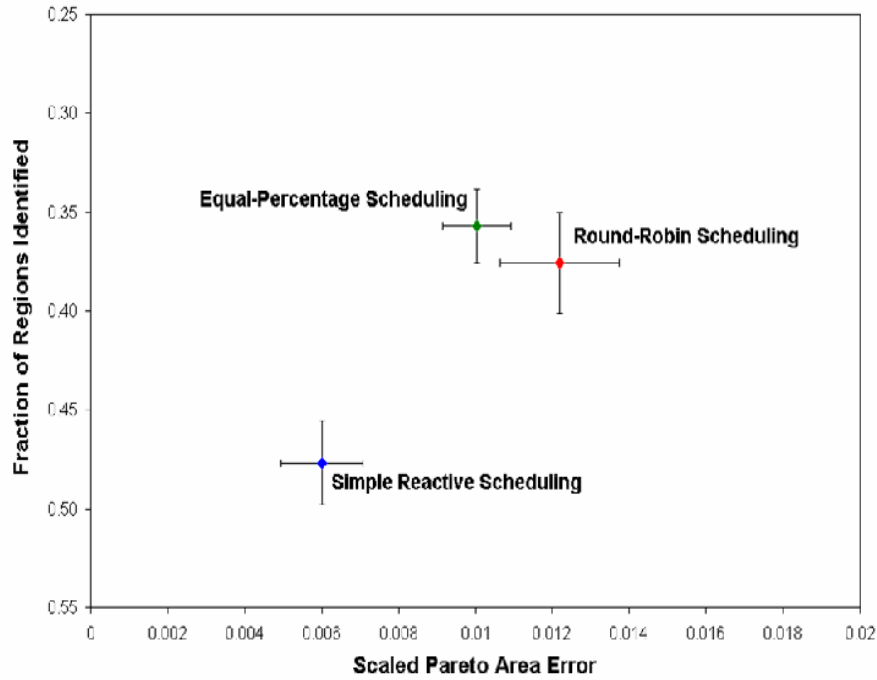
1. The master resource control loop determines the individual agents' access to computing power. With the assumption that the number of possible cases to run is substantially larger than the available resources, selecting a promising agent-pool with sufficient variability becomes a crucial step in solving large problems.

2. All solution agents are divided into two parts: The preprocessing--or 'scouting'--step analyze the current state of the problem and estimates a probability of improvement. This is fed back to the resource control agent, which may or may not decide to allow the actual 'work' part of the agent to be run. A key point is that not all agents are expected to yield actual solutions; it is perfectly acceptable to use heuristic or statistical rules to deduce, suggest or guess where good solutions may -- or may not -- be found.
3. The meta-agents analyze the performance of the pool of solution agent. This is fed back to the resource control loop to help divide the problem into solution 'phases' and to minimize the waste of resources on agents not suitable for the problem at hand.

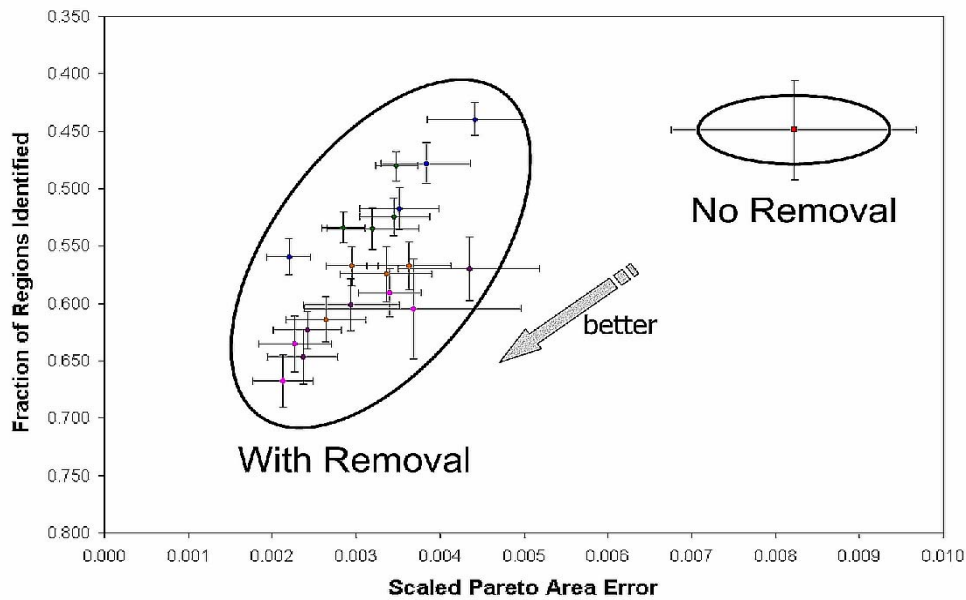
PROGRESS

John's time over the last 4 months have been spent working on two fundamental operation and management issues in multi-agent system design: agent scheduling and shared memory management. Previous work used a very simple agent scheduling policy with constant, equally-divided agent populations. We have tested a number of different schemes for resource allocation and demonstrated that significant improvements of solution quality is possible. The main idea is that a path toward the final set of solutions go through different phases; each of which have their own "optimal" distribution of CPU resources between different agent types. This is currently implemented in a simple feed-forward control loop where agents that recently contributed to improving the current pareto-solution receive a boost in their expected resource allocation. The effect is schematically illustrated in the figure above where the adaptive resource allocation scheme is labeled "Simple Reactive Scheduling."

Effective policies for managing the shared memory system are also critical for developing effective multi-agent systems. In previous work, we focused primarily on problem-solving agents that strive to generate new solutions to the problem. The solutions generated by these agents accumulated in the shared memory system throughout the simulation. For relatively short simulations, these agent sets performed very well. However, larger and longer-running simulations rapidly reach a point where the shared memory system becomes a bottleneck, significantly slowing the problem-solving agents' ability to generate new solutions. Removing solutions from the shared memory can alleviate the bottleneck so that the memory size does not reach the point where it significantly limits the database server's ability to return information. The effect of solution removal is illustrated in the figure below and show that solution quality may nearly doubled with constant computational efforts by proper solution removal policies.



Effect of agent allocation scheduling



Effect of Limiting the Size of Shared Memory

The agent system is currently being applied to the generation of layout for chip-based electrophoretic separation systems.

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 (PhD, started Jan 2002) and Xiang He (MSc, starting Jun 2003)

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

BACKGROUND

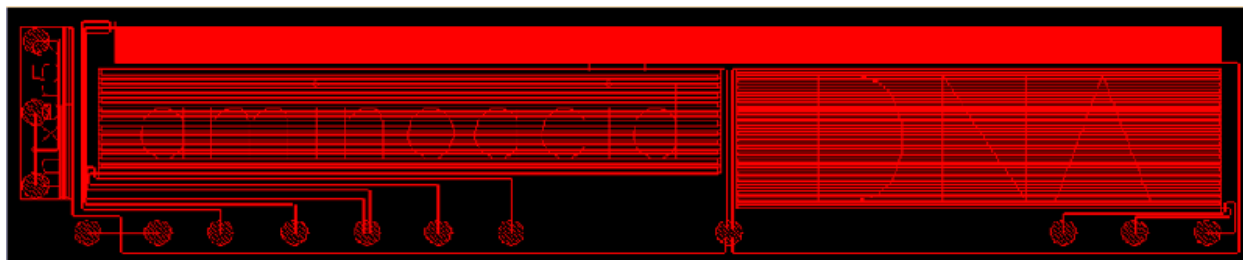
Microfabrication process have enabled manufacture of micro-sized channels, pumps, valves, mixer components and reactors. Integration of these components have enabled the creation of on-chip systems that span sample collection, preparation and analysis of biological materials, drug screening and chemical 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 customized BioMEMS devices where multiple microfluidic components are tailored to suit individual performance requirements.

PROGRESS

Anton has spent most of his time this fall on two projects: (1) a DARPA design challenge for integration of multiple separation subsystems on a single glass chip, (2) preparation for his PhD proposal exam and talks at the annual conferences for chemical (San Francisco) and mechanical (Washington DC) in November.

The result is shown in the figure below. There are 4 independent subsystems in the design; all achieving a component separation sufficient to discriminate between individual species in what starts out as a multicomponent mixture. The systems are: (1) a collection of 20 amino acids, (2) a common mixture of 10 peptides, (3) a set of 50 similar DNA fragments, (4) a mixing/reaction system for molecular tagging.



DARPA Design Challenge: On-Chip Separation with 4 Subsystems

The methods used were presented at the AIChE annual meeting (San Francisco, November) and at the equivalent mechanical engineering meeting (IMECE '03, Washington DC, November) and was made available in a preprint distributed in the Aug 2003 copy of the CAPD newsletter.

(b) A MEMS-based Gravimetric Biosensor

Students: Michael Bartkovsky (PhD, started Jan 2002), Jane Valentine (PhD, started Jan 2003),

Collaborators: Todd Pryzbycien (Biomedical Engineering), Kaigham Gabriel (ECE), John Neumann (ECE)

BACKGROUND

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

There are four major tasks in this project:

- (a) fabrication of a CMOS/polymer membrane with integrated capabilities for actuation and capacitive sensing.
- (b) chemically specific functionalization of the membrane surface such that target molecules get adsorbed with the highest possible selectivity

- (c) creating a clamshell packaging in which liquid samples may be brought in contact with the membrane surface.
- (d) computer aided optimization of system parameters – including device geometry, functionalization density and scanning frequencies -- for single membranes as well as arrays of such.

PROGRESS

The main progress in this project has been to identify and test experimental protocols for chemical functionalization of polymer surfaces (Mike) and to establish physically reasonable bounds for "detectability" (Jane) for target molecules in the original sample, in the liquid streams being processed and "near" the functionalized surface. On the experimental side, crosstalk between the actuation and sensing elements in the MEMS chip has so far made electronic measurements in liquid impossible. Although a microvision system for optical detection is being configured, all-electronic detection is being addressed with embedded piezoelements for the next generation design. A number of simulations for vibrating membranes have been carried out to assess the spatial sensitivity to mass loading for multifunctional membranes. The results show that "proper" positioning of binding sites on the membrane surface lead to order of magnitude improvements in sensitivity with respect to the amount needed to identify a positive response. At present we are trying to formulate the inverse problem where we not only aim to identify the optimal approach to surface functionalization, but also seek to maximize the robustness to non-specific binding and low concentration of target molecules.

A patent application (US and International) entitled "A MEMS-Based Biosensor" was submitted in November.

Erik Ydstie's Group

Distributed Simulation and Control of Process Networks

Students: Vianey Garcia-Osorio (PostDoc May 2003-June 2004)

Vianey Garcia-Osorio developed a new approach for static and dynamic simulation of process networks in her PhD studies. She tested the approach for a simple recycle problem and a preliminary model of a carbothermic aluminum process. The simulation approach is carried out in parallel over the web and can lead to significant improvements in computational speed and savings in development cost. The current method is implemented in MATLAB/SIMULINK. One unique aspect of Vianey's approach is that the method does not require a central coordinator to stabilize the computation. In this way the simulation is scale-able and very large systems can be simulated without slowing down the execution speed. Inher current PostDoc work she is refining the method, developing stability theory and she is also investigating the application of real time optimization methods to improve process design. Part of this work is funded by ALCOA and one important aim of the study is to aid in the development of model systems for pilot plant and conceptual desing.

Adaptive Enerprise Systems

Students: Kendell Jillson (PhD)

The objective of this research is to develop models for highly distributed and adaptive enterprise systems. In this research we use stability results for process networks that Duncan Coffey's (PhD 2001) developed. Kendell Jillson is continuing this work. But his work focuses on optimality properties of large integrated networks of process systems. He has developed optimality results for tow types of static networks. Using a version of Tellegen's theorem form circuit theory he has shown that distributed systems with positive cost relations automatically balance load so that that the activity costs are minimized. In the linear case this result shows that the network automatically solves Linear and Quadratic programs. He is currently looking at stability properties of such networks and he is also developing a range of case studies to test and develop the methods further.

Modeling and Control Complex Chemical Reactors

Students: Dimitrios Gerorgios (PhD)

Vianey Garcia-Osorio (PostDoc)

Berit Floor Lund (PhD University of Trondheim, Norway)

We have developed models for distributed parameter systems that can be used for conceptual design and control studies. The aim is to develop a unified framework for modeling simulation control and optimization of systems that integrate fluid flow, particulate matter, and chemical reaction.

Dimitrios Gerorgios is developing a Computational Fluid Dynamics (CFD) model of multi-phase reaction with electrical fields. The system we develop is used for conceptual design of a new process for carbothermic reduction of alumina to make aluminum. The model system operates at elevated temperatures around 2000°C and includes a fluid/gas/solid CFD model for the electrical fields, fluid flow, and chemical reaction. His new model includes the formation of bubbles using a two phase flow approximation.

Vianey Garcia-Osorio continues to develop models the vapor recovery section of the aluminum process. A significant amount of aluminum vaporizes from the aluminum reactor and this aluminum must be recovered in a vapor recovery column. Vianey models the primary reaction in the column, the gas flows as well as solid transport. Her focus is to develop efficient methods to represent the thermodynamics and the multiphase behavior of the VRR. This work is now concluded and we are finishing up a three phase (liquid/solid/gas) simulation model which will be used for system design, economic evaluation and control studies.

Berit Floor Lund (University of Trondheim, Norway. Advisor in Norway, Bjarne Foss). Berit continued Martin's study of the Silicon reactor control and optimization study. She concluded a dynamic study of the behaviour of the zero dynamics of the reactor which will be published in the INFACON progress. This study included sensitivity results for the reactor and critical parameters for standard operating conditions. Berit also developed a new method for parameter estimation.

Modeling and Control of Particulate Processes

Students: Christy White (PhD)

Marta Duenas Diez (PhD Telemark)

The Photovoltaic industry is facing a critical shortage of solar grade Silicon and a large number of manufacturers world wide are trying to develop new production technology to meet the demand in a market that continues to grow at a rate of 35-30% annually. We have started an investigation aimed towards the development of new fluid bed decomposition of Silane in a closed reactor, separator system to produce high purity silicon for solar cells. Christy White has developed a population balance model to represent the static and dynamic behavior of the process. The model will be matched to data supplied by SGS LLC. Once she has developed a reliable model she will address problems related to process control and optimization for this new process. She is in particular interested in developing methods that can be used to predict and control the particle size distribution.

Marta has developed simulation models and inventory control methods for particulate processes. She is developing a case study for the ELKEM Silgrain process which produces 80% of all Silicon for the Japanese semi-conductor industry. Marta has tested the use of inventory control to stabilize this process and she has been getting very good results that were presented at the AIChE meeting. Her models have now been verified industrially and she has been able to show that the two compartment model gives realistic prediction of particle size distribution. We plan to generalize the concept to a broader class of problems, including biological systems and crystallization processes.

Thermodynamics and Process Networks

Students: Luis Antelo

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.

Real Optimization of Silicon Reactors

Students: Jin Wang (PostDoc)

Jin Wang has developed a simple version of Martin Ruzskowski's model for the primary silicon production unit at the ALLOY plant. The primary reactions, which take place between silicon, silicon dioxide, and silicon carbide are modeled using simplified kinetic expression with transport and reaction coefficients matched to the process on-line. We have used this model to develop new control strategies for nonlinear control and real time optimization. Jin has also developed a new method for constrained state and parameter estimation which looks very promising in simulation studies.

PUBLICATIONS

B-03-05

Poku, M. B., J. D. Kelly, L. T. BIEGLER, “Nonlinear Programming Algorithms for Process Optimization with Many Degrees of Freedom,” submitted for publication (2003)
<http://dynopt.cheme.cmu.edu/papers/preprint/paper24.pdf>

B-03-06

Borrelli, F., D. Subramanian, A. U. Raghunathan, L. T. BIEGLER and T. Samad “A Comparison between Mixed Integer Programming and Nonlinear Programming,” submitted for publication, Proc. American Control Conference (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper25.pdf>

B-03-07

Raghunathan, Arvind, M. Soledad Diaz, Lorenz T. BIEGLER “An MPEC Formulation for Dynamic Optimization of Distillation Operation,” submitted for publication, (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper26.pdf>

B-03-08

Xu, C., P. M. Follmann, L. T. BIEGLER and M. S. Jhon, “Numerical Simulation and Optimization of a Direct Methanol Fuel Cell” submitted for publication (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper27.pdf>

B-03-09

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,” submitted for publication (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper28.pdf>

B-03-10

Jiang, L., V. G. Fox and L. T. BIEGLER, “Simulation and Optimal Design of Multiple-bed Pressure Swing Adsorption Systems,” submitted for publication (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper29.pdf>

B-03-11

Kameswaran, S., G. Staus and L. T. BIEGLER, “Parameter Estimation of Core Flood and Reservoir Models,” submitted for publication (2003) <http://dynopt.cheme.cmu.edu/papers/preprint/paper30.pdf>

G-03-04

Balasubramanian, J. and I. E. GROSSMANN, “Scheduling Multistage Flowshops with Parallel Units -An Alternative Approach to Optimization under Uncertainty,” submitted for publication (2003).
<http://egon.cheme.cmu.edu/Group/Papers.html>

G-03-05

Caballero J.A. and I. E. GROSSMANN” “General Design Of Distillation System: From Conventional To Thermally Coupled Distillation Systems,” submitted for publication (2003). <http://egon.cheme.cmu.edu/Group/Papers.html>

G-03-06

Ghosh, S., T. Zhu, I.E. GROSSMANN, M.M. Atai, and M.M. Domach, “Closing The Loop Between Feasible Flux Scenario Identification For Construct Evaluation & Resolution Of Realized Fluxes Via NMR,” submitted for publication (2003). <http://egon.cheme.cmu.edu/Group/Papers.html>

G-03-07

GROSSMANN, I.E., “Challenges in the New Millennium: Product Discovery and Design, Enterprise and Supply Chain Optimization, Global Life Cycle Assessment. <http://egon.cheme.cmu.edu/Group/Papers.html>

G-03-08

Maravelias, C.T. and I. E. Grossmann, “A General Continuous State Task Network Formulation for Short Term Scheduling of Multipurpose Batch Plants with Due Dates,” submitted for publication (2003).
<http://egon.cheme.cmu.edu/Group/Papers.html>

H-03-04

Siirola, John D. and Steinar Hauan. RPI: A Remote Process Interface library for distributed clusters; Submitted to *Comp.Chem.Engng.*, Dec. 2003. <http://www.andrew.cmu.edu/user/steinhau/Publications/>

Y-03-01

Lund, Berit F., B.A. Foss, K.R. Lovasen and B. Erik Ydstie, "Analysis of Carbon Coverage to Silicon Taprate Dynamics in a Submerged Arc Silicon Furnace," supported by NTNU and Elkem, 2003.

Y-03-02

Ydstie, B. Erik, "Passivity Based Control via the Second Law," supported by NSF, Alcoa, Inc. and Elkem Foundation, 2003.

REPRINTS

Gerogiorgis, Dimitrios I. and B. Erik Ydstie, "Flow Modeling for Design of Carbothermic Aluminium Reactors," *Third International Conference on CFD in the Minerals and Process Industries*, CSIRO, Melbourne, Australia, 10-12 December 2003.

Grossmann, I.E. and S. Lee, "Generalized Disjunctive Programming: Nonlinear Convex Hull Relaxation and Algorithms", *Computational Optimization and Applications* **26**, 83-100(2003).

Jockenhoevel, T., L. T. BIEGLER and A. Waechter, "Dynamic Optimization of the Tennessee Eastman Process Using the OptControlCentre," *Computers and Chemical Engineering*, **27**, 11 pp 1513-1531 (2003).

Perea, E., E. Ydstie and I.E. Grossmann, "A Model Predictive Control Strategy for Supply Chain Optimization," *Computers and Chemical Eng.*, **27**, 1201-1218 (2003).

Raghunathan, A. U., J. R. Pérez-Correa and L. T. BIEGLER, "Data Reconciliation and Parameter Estimation in Flux-Balance Analysis," *Biotechnology and Bioengineering*, **84**, pp. 700-709 (2003)