TABLE OF CONTENTS

GENERAL NEWS

The National Science Foundation has awarded two Information Technology Research (ITR) Grants to CAPD investigators. These awards will provide over two million dollars of funding over the next five years, primarily for graduate student support. The first grant on *Model-Based Integration of Methods for the Optimization of Process Systems* is awarded to **Ignacio Grossmann** and John Hooker (GSIA) at CMU. The second grant on *Real Time Optimization for Data Assimilation and Control of Large Scale Dynamic Simulations* is awarded to **Larry Biegler** and Omar Ghattas (CEE) at CMU. Both grants are devoted to research in optimization methods and engineering applications. We also believe that these grants will be an excellent opportunity for CAPD members to leverage their research interests in process systems engineering.

Lee Sangbum and Ignacio have won the 2000 Best Paper Award in Computers and Chemical Engineering, "New Algorithms for Nonlinear Generalized Disjunctive Programming," *Computers and Chemical Engineering*, **24**, pp.2125-2141(2000).

Iiro Harjunkoski, who was a postdoc working with Ignacio, has joined ABB in Heidelberg, Germany, to develop optimization models for planning and scheduling.

Mariana Barttfeld, from INGAR in Santa Fe, has joined Ignacio's group for one year. Mariana, who is doing her Ph.D. under the direction of Dr. Pio Aguirre in Argentina, will be working in the area of synthesis of separation systems.

Art and Ignacio have participated in the Roger Sargent Symposium at Imperial College in London, in occasion of Sargent's 75th birthday.

NEW STUDENTS

We are pleased to announce that the following new students have joined CAPD research groups: **Carl Laird** (University of Alberta) and **Shivakumar Kameswaran** (IIT Madras) joined Larry's group; **Nikolas Sawaya** (McGill, Montreal) and **Soumitra Ghosh** (IIT Karagpur) joined Ignacio's group; **Anton Pfeiffer** (University South Florida) and **Michael Bartkovsky** (University Pittsburgh) joined Steinar's group; **Luiz Felipe Tavarez** (University Rio de Janeiro) joined Erik's group as a M.S. student; **Miguel Vescovacci** (University Puerto Rico) joined Gary's group as a M.S. student.

FOCAPO 2003

Ignacio will be co-chairing together with Conor McDonald the FOCAPO (Foundations of Computer Aided Process Operations) 2003 Meeting that will take place on January 12-15, 2003, in Coral Springs, Florida. The theme of the meeting is "A View to the Future Integration of R&D, Manufacturing and the Global Supply Chain." Information about this meeting can be found in http://www.cheme.cmu.edu/focapo. We also enclose a flyer describing this meeting. We expect that this meeting will attract many industrial practitioners. We hope you will be able to submit a contributed paper. The deadline is March 1, 2002.

2001 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on ***April 2-3, 2002***. This is on Tuesday and Wednesday of spring break. The first day of the meeting consists of overviews given by principal CAPD researchers, followed by a discussion with industrial participants, a poster session by the students, and a group dinner. A very successful group dinner was held last year at the Monterey Bay Fish Grotto. The second day will be devoted to final year student presentations and a wrap up session. We are especially grateful for the very

positive feedback on last year's meeting. If you have any additional thoughts or suggestions for this year, please let us know.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* will be offered on June 20-26, 2002. We were very pleased with the outcome of our last course. We had 11 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 (June 20-21), 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 (June 22 and 24), 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 (June 25-26), 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 includes extensive workshops where participants obtained hands-on experience with various software packages. Course materials included extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in attending this course next summer, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that this issue of the CAPD newsletter, including the reprints and papers, will be distributed in electronic form. All members will have access to these items via our web page, http://www.cheme.cmu.edu/research/capd/.

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 the updating of 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

Highlights of **Larry Biegler's group** include further development of the reduced Hessian SQP (rSQP) strategy along several directions. The FORTRAN version of the rSQP strategy has been used for optimization of black box units including PDE based models involving convection and diffusion. Examples of this include CVD reactors (**Greg Itle**), PSA systems (**Ling Jiang**) as well as other fluid flow systems (**Cong Xu**). Moreover, **Andreas Waechter** is developing and refining a barrier (interior point) NLP method, called IPOPT, based on many of these SQP concepts. This has been used to solve problems with rSQP that incorporates a number of specialized decomposition strategies and high levels of abstraction for a wide variety of applications. Finally, **Roscoe Bartlett** completed his PhD in August and 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. Both IPOPT and rSQP++ will be available under Open Source software licenses and more information on distribution will be in the next newsletter.

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 through an ftp server. Please contact lang+@andrew.cmu.edu or biegler@cmu.edu for more information. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package will be enhanced further by incorporating the ESO CAPE-OPEN modeling standards currently used in gProms. In a parallel, effort we are working with researchers **Tobias Jockenhoevel** and **Yuen Yee Jin** from the Technical University of Berlin on the OCOMA package, which incorporates these dynamic optimization strategies using MATLAB interfaces. In addition, two postdoctoral visitors, **Daeho Ko** and **Masaru Noda**, and a faculty visitor, **Ricardo Perez**, are working on applications of dynamic optimization of large scale systems. Daeho is working on PSA optimization for CO2 capture; Masaru is working on fuel cell optimization and Ricardo is addressing the optimization of cellular systems.

In the area of reactor network synthesis, **Bill Rooney** and **Shehzaad Kauchali** have developed a new linear programming based algorithm for the construction of attainable regions. In addition, for his PhD thesis, Bill modified the flexibility approach of Grossmann and coworkers to deal with uncertainty associated with nonlinear model parameters. This strategy incorporates nonlinear confidence regions into the uncertainty description in an efficient way and leads to a more realistic characterization of the impact of model uncertainty. He has also extended this to problems where uncertainty falls into two categories: one that is compensated by feedback and another that requires a robust design. Finally, **Nikhil Arora** has demonstrated the use of efficiently derived M-estimators for data reconciliation problems and gross error detection. These approaches are statistically tuned using the Akaike Information Criterion and perform very well compared to combinatorial approaches. Currently, he is developing a robust NLP algorithm for this class of problems.

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

In the area of process synthesis **Jennifer Jackson** has been working in a multisite multiperiod optimization planning model that makes use of process models. This project has been motivated by a collaboration project with Dow Chemical. We enclose a copy of a paper on the earlier work she did for retrofit planning. **Mariana Barttfeld**, who has recently joined our group, has been comparing alternative MINLP and disjunctive formulations for distillation column design, as well as coupling these models with effective initialization schemes developed by her and Pio Aguirre at INGAR in Argentina. **Jose Caballero** in Alicante is also helping in this effort by looking at superstructures for thermally integrated columns.

In the area of optimization **Sangbum Lee**, has developed a specialized version of his global optimization method for generalized disjunctive programming models to rigorously handle bilinearities that arise in process networks (eg. pooling, separation, water treatment). This work builds on previous work by Quesada

who addressed the question of compositions versus individual flows models for global optimization. **Aldo Vecchietti**, is completing the version of LOGMIP for handling disjunctions with linear constraints.

In the area of planning and scheduling **Jayanth Balasubramanian,** has completed the work on a new approach for scheduling under uncertainty that relies on concepts of interval arithmetic and fuzzy sets and numbers. He has applied it to flowshop scheduling problems and to the new product development problem, requiring orders of magnitude faster than alternative probabilistic methods. **Iiro Harjunkoski** completed the work for a hybrid scheme (MILP and Constrained Programming) for multistage batch scheduling. A copy of the paper describing this work is enclosed in which examples are presented that lead to order of magnitude reductions in computations. **Christos Maravelias** has completed the work for simultaneous scheduling for new product development and batch plant design. As part of this project he has been investigating new formulations and efficient solution methods for the resource constrained scheduling problem for new product development. Initial results indicate that a logic-based approach that uses implied precedences can have a large impact for reducing the computational time. **Martin Houze** has been able to obtain comprehensive results with a multiperiod MINLP model on a project that is in collaboration with TOTALFINAELF in the area of optimal catalyst management. In the area of supply chain optimization, **Edgar Perea,** under the supervision of Ignacio and Erik, has continued to develop in collaboration with Unilever a Model Predictive Control algorithms that reduces to solving a sequence of MILP problems for supply chain optimization. He has found that economic optimization yields superior results, compared to a decentralized control approach. Finally, **Gabriela Garcia** is close to completing the transfer of the interface WATER to a web-based system in which GAMS is automatically invoked.

In **Steinar Hauan's** group, **Warren Hoffmaster** continues to work on the feasibility analysis and design of reactive separation processes with special focus on distillation. Several interesting discoveries have been made, including the theoretical bounds for a single cascade section with simultaneous reaction and separation as well as fold points in the kinetically controlled reactive phase space. Warren has also completed a paper on the analysis of reactive cleanup columns to avoid recycle in the production of acetic anhydride.

John Siirola, working with **Steinar Hauan** and **Art Westerberg**, has completed a first manuscript in which he demonstrates the synergy of using many types of collaborating agents to solve complex optimization problems. He repeatedly optimized (to build up "average" performance of the approach) a problem having 1017 local optimum, with 10 equal global optimal, using differing agent combinations. Multiple, diverse agent systems often found all ten global optimum. Using the same total computer resources, single agent systems always stalled far from any of the global optimum. The tests show clearly the impact of the collaboration among the agents on algorithm performance and is implemented in a scalable fashion.

Murni Ahmad has been working with **Todd Przybycien** on flexible design of biochemical processes. She will finish her MSc thesis on modeling of 2-phase aqueous system for protein separation and will continue on in the group with a PhD. Two new students have just joined the group this month. **Anton Pfeiffer's** project deals with the synthesis of chip-based detectors based on electrophoresis and involves theoretical and experimental work by collaborators in ECE and ME. **Michael Bartkovsky** (co-advised by Todd) will be working on microscale gravimetric detectors based on polymer membranes on a chip.

Fabio Mizutani, a visitor from University of Rio (Brazil), has developed a mathematical programming formulation for heat exchangers that incorporates detailed sizing and costing of individual units. A sequential network model has been developed and work in progress aims to convexify the formulation as well as extending it to simultaneous solution of structure and individual exchangers.

Our Beowulf computer cluster is now a 64-cpu system and facilities are being upgraded to house a January expansion.

In **Gary Power's** research group, the research on the verification of a complex control system for the casting of metals is continuing. Ph.D. candidate **Mr. Dan Milam** is developing a modeling system for modular models that can be assembled into a systems model that can be verified against operability and safety specifications for the process. **Mr. Dan Margolis** is building a system for writing and verifying operating procedure systems.

These researchers have been working with an industrial team that has been developing and installing the control system. The models of the system have been developed in a staged manner that allows for the capture of faults at the conceptual and more detailed stages of the design. Methods for capturing the information required from the design and converting it into a model appropriate for verification are being developed for relay ladder logic diagrams, C++ programs and operating procedures.

The faults discovered by the verification are being compared with those detected by the normal startup testing.

In **Art Westerberg's group**, **Lifei Cheng** continues his work to create a simulation/ optimization/ design/ operation capability for stochastic models that describe the long-term future behavior of a process. He describes this work in a paper circulated with this newsletter. In it he shows how to formulate a problem with multiple objectives so it can be properly decomposed using a dynamic programming based algorithm. He also demonstrates, with a small problem, the very significant impact on solutions one will find that trade off present worth and risk.

A visiting faculty member, **Zhijiang (Jon) Shao** from Hangzhou, China, is a month from completing his half year stay. He has developed a set of tools to allow one to develop and solve MATLAB equation-based models in the "ASCEND" style.

Erik Ydstie's research group continues to work on process control and dynamic simulation of complex chemical process. We work on *plant wide process control, supply chain management, modeling, optimization g and control of distributed process systems and adaptive process control and optimization* and stability analysis of process networks. A special decomposition method links the process network problem with circuit theory and this allows us to develop a rather complete theory for plant-wide process control. A brief summary of progress made in each of these areas is given below.

We have showed that the multi-component *distillation* process is open loop stable. This is an important result and the first stability result to appear in this area since the stability result due to Rosenbrock in 1964. Rosenbrock's result is only valid for binary systems and his method of proof cannot be extended. Our approach is based is based on the general theory of process systems and it can be extended to heterogeneous and reactive systems. We do believe that a stability result for reactive distillation is valid as long as the reactions are close to equilibrium.

We made significant progress on the problem of parameter drift and bursting in *adaptive control*. An algorithm which only uses the most reliable data for parameter estimation has been developed. We have shown that the method converges an that that it yields models that can be arbitrarily close to the optimum under very mild conditions. We have implemented the method in the context of adaptive predictive control and it has tested it on a simulated PPG case study for glass temperature control. We have also developed an adaptive predictive controller of crown temperature in SIEMEN's glass furnaces. This controller has been implemented on an industrial furnace and has been in continuous operation for about two years. We are now working on the problem of extending her theories and methods so that they can applied for large scale production of Silicon in electric arc furnaces.

We are developing systematic methods for modeling large scale chemical processes. The method uses a decomposition scheme and strict rules for model interconnectivity that allow us to proceed in a modular fashion and also to simulate the systems statically or dynamically over the web in a distributed network of computers. We are currently working on two case studies funded by industry. With ALCOA we develop a

design model for a new Aluminum process. The process is based upon carbothermic reduction rather than electrolysis. It may give significant savings in operating and capital cost. With ELKEM we develop a dynamic model of the their Silicon production process. This model will be used for control design and real time process optimization.

The research group has re-initiated its interest in discrete event systems and we have two projects in the area of *supply chain management*. One of these are carried out in cooperation with Prof. Grossmann's research group. The other project is aimed towards generating a deeper understanding of the optimality and invertibility properties of the desk-top problem.

Finally we are continuing our research in linking thermodynamics and process control. The foundation is based on a the convexity property of the entropy function and the implications that this has for stability analysis, optimization and control of chemical process systems.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

rSQP++: A Framework for Large Scale Optimization Strategies
Student: Roscoe Bartlett (Ph.D. student completed August, 2001)
Carl Laird (Ph.D. started Fall, 2001)

Roscoe Bartlett completed his PhD in August and has taken a position at Sandia National Laboratory in Albuquerque, NM. For his thesis he has developed and thoroughly tested an object oriented version of rSQP written in C++. This version allows the easy incorporation of options, Hessian classes, different linear algebra and QP solvers, as well as dynamic memory allocation and management. This approach makes extensive use of mixed language programming so that the 'number crunching' parts are handled by FORTRAN (and mostly BLAS) routines while the higher level code is in C++. To do this work, Roscoe has developed a comprehensive structure for linear algebra. Currently, he is extending these linear algebra classes to support a high level of abstraction for diverse solver environments including: dense LINPACK solvers, sparse direct solvers, iterative preconditioned Krylov solvers and computing in parallel environments. In particular, these will make use of a number of large-scale linear solvers including PETSc at Argonne National Lab and Petra at Sandia National Labs.

In addition, Roscoe has developed rSQP methods based on the application of Schur complements for the active set strategy in the QP. This approach has been very successful for the SOCS code at Boeing. Unlike the QPKWIK algorithm, the application of Schur complements allows us to directly exploit the structure of the entire KKT matrix at the linear algebra level. When applied to standard NLP test problems, this new Schur complement QP approach (called QPSchur) is at least three times faster than QPKWIK and about an order of magnitude faster than QPOPT on unstructured problems. As a stand-alone QP package, QPSchur has been compared against QPKWIK, QPOPT, LOQO and the MATLAB QP code on large-scale problems in Model Predictive Control (MPC). This problem, with up to 600 inputs was based on the cross-directional control of a paper machine. For this test problem, QPSchur was at least an order of magnitude faster than any of the competing codes. Moreover, with the application of QPSchur we were able to demonstrate that the on-line solution of MPC controllers based on quadratic programming is indeed feasible for these challenging processes. A paper that describes this comprehensive comparison is listed below. A detailed description of QPSchur can be found in Roscoe's thesis and a publication describing this method is currently in preparation.

As a result, a general active set strategy can be developed for very efficient NLP algorithms for rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. The resulting package, rSQP++, has recently been adopted by Sandia National Labs as their framework for large-scale PDE-based optimization problems. Roscoe is currently working in interfaces to a number of sophisticated PDE

packages including MP/SALSA and GOMA at Sandia. A paper that describes this approach in some detail is currently in preparation and will be distributed with the next newsletter.

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. For this purpose, we have considered linear model predictive control problems and large dynamic optimization problems for NMPC. In the former case, Roscoe showed that QPSchur is very efficient on these problems, particularly if the number of inputs is large. For the latter case, we are interested in knowing when barrier approaches (see below) are favored over active set strategies. We have applied both approaches for the full-scale Tennessee Eastman problem and noted the following features:

- for problems with many states and few controls, a reduced space approach has significant advantages over NLP methods with full space decomposition. This is often due to limitations of current sparse linear solvers

- for problems with few active constraints a well implemented active set strategy still has advantages over barrier methods. These advantages disappear as the number of active constraints increases.

Finally, extensions of rSQP++ will be made for multiperiod optimization and optimization under uncertainty. In addition, we will expand the functionality of this code to consider interior point solvers. Carl Laird has recently joined the group and will be working on these extensions.

Large-Scale Optimization for Partial Differential Equation Models
Students: Gregory Itle (Ph.D. student started Fall, 1998)
Cong Xu (Ph.D. student started Fall, 2000)

Gregory Itle is extending tailored rSQP concepts into the area of optimization of systems described by partial differential equations. Working with researchers at Sandia National Lab and with Prof. Omar Ghattas and his group, he is applying NLP strategies to finite element models for fluid flow, heat and mass transport and reaction in distributed domains. In particular, he has recently developed a prototype interface of the FORTRAN version of rSQP with MP SALSA, a large-scale partial differential equation solver. This was demonstrated on the optimization of a natural convection system. Currently, he is streamlining and applying both the FORTRAN rSQP code and rSQP++ to adapt it to larger NLP problems for nonideal reactor applications. For this topic Greg is also looking at constraint aggregation strategies that allow much less overhead to constraint activity and also allow conventional QP solvers to be used even if there are millions of bound constraints. Greg is currently working at Sandia to implement and test these ideas.

During the past six months, Greg applied this approach to the optimization of a Chemical Vapor Deposition (CVD) reactor. Modeled as a finite element problem in MP SALSA, this application leads to an optimization problem where we maximize the uniformity of the wafer thickness by manipulating operating and geometric decisions in the reactor chamber. For this problem, the rSQP optimization algorithm takes full advantage of the finite element meshing, initialization and large-scale iterative solvers in MP SALSA and has also been run on parallel processors. Because, the tailored rSQP approach allows simultaneous convergence and optimization, it allows the CVD optimization to be run about an order of magnitude faster than with standard black box solvers. Greg is extending this approach to include rSQP++ and to larger problems with three dimensional flow fields. In addition, he is considering novel constraint aggregation strategies for problems that are very highly constrained within these flow fields. He is also exploring trust region strategies and the use of KS functions to aggregate large numbers of inequality constraints that occur in these optimization problems. In doing so, the QP subproblem becomes much smaller and faster to solve. A paper that describes this approach is currently in preparation and will be distributed with the next newsletter.

Finally, Cong Xu recently passed his PhD qualifier and is investigating optimization problems arising in fluid dynamics and transport phenomena using Smooth Particle Hydrodynamics (SPH). Currently, he has developed a particle based CFD code that requires the solution of DAEs rather than PDEs. Also, he is evaluating SPH for a number of fluid flow applications including flows in complex geometries and limits of compressible flow. Our intention is to extend this approach to consider sensitivity and optimization calculations for these models.

Barrier (Interior Point) Methods for Nonlinear Programming

Students: Andreas Waechter (Ph.D. student started Fall, 1997)

This project considers the development of an efficient strategy for solving nonlinear programs using interior point (IP) methods. This approach works either in the full space or can take advantage of the particular rSQP decomposition strategies (choices of Z and Y) 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 started by adapting the algorithms of Byrd and Nocedal to specialized characteristics encountered in process engineering optimization problems. A number of variations to this approach have been developed and tested 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 through analysis of this difficulty. A reprint of the paper that discusses this phenomenon is listed below. 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. A manuscript that describes the filter method along with a local and global convergence analysis is listed below. Numerical testing on over 300 test problems has also shown some significant performance improvements over other barrier algorithms. Major features of this approach are:

- an implementation that combines Cauchy and Newton steps for the range space move and avoids the problem described in the paper below
- 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.

To test these ideas, a FORTRAN code has been implemented for the solution of dynamic optimization problems; problems with over 1,800,000 variables have been solved in a few hours of CPU time on an 700 MHz computer. Moreover, this approach has been linked to a number of packages including DynoPC, OCOMA and AMPL. Finally, an open source license is being prepared for this code and more details on the distribution of IPOPT will be described in the next newsletter.

Mathematical Programs with Equilibrium Constraints (MPECS)

Students: Arvind Raghunathan (Ph.D. started Fall, 1999)
Maame Poku (Ph.D. started Fall, 2000)
Shivakumar Kameswaran (Ph.D. started Fall, 2001)

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. Preliminary work in this area includes the following:

Arvind Raghunathan has incorporated the MPEC formulation into the IPOPT code 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. Preliminary 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. Preliminary 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 conditional relationships using complementarity conditions instead of binary decision variables. While this leads to nonconvex NLPs, the solution of these MPEC problems can lead to satisfactory solutions with less computational effort than in solving MINLPs.

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. Preliminary results show that the full-space version of IPOPT works quite well on these problems.

Future work will deal with a more general development of MPEC formulations and solution algorithms. In addition to phase equilibrium problems, we will consider hybrid systems with a limited set of discrete decisions that can be modeled as monotone complementarity problems. This is especially important since convergence properties for barrier methods have already been shown for these problems. In addition, Shivakumar Kameswaran has recently joined this project and will be applying the IPOPT-based strategy to large-scale process operations problems formulated in AMPL.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Students:	**Arvind Raghunathan (Ph.D. started Fall, 1999)**
Researcher:	**Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Visitors:	**Tobias Jockenhoevel and Yuen Yee Jin (Technical University of Berlin)**
	Prof. Ricardo Perez (Potifical University of Chile)
	Dr. Masaru Noda (Kyoto University)

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 finite elements as well.

In previous work, Arturo Cervantes developed and expanded the simultaneous approach to solve moderately large dynamic optimization problems. This is being accomplished through the incorporation of more efficient matrix decomposition strategies, with COLDAE routines to set up the collocation equations. In addition, Arturo has solved a number of process optimization problems including the dynamic optimization of reactive distillation columns, polymerization reactors and crystallization units. This work covers two areas. First, with Prof. J. A. Bandoni and his colleagues at PLAPIQUI in Bahia Blanca, Argentina we refined an optimization model for a LDPE reactor. The dynamic optimization problem deals with shortening the grade transition time from one set of operations to another. Application of the above strategy led to an optimization of a DAE model with over 200 DAEs in less than 10 CPU minutes. As a result, the transition time for this reactor was shortened from five to two hours. This model has also been extended to incorporate reactor kinetics and consists of over 530 DAEs.

For these large-scale optimization algorithms, it is essential to develop modeling environments that allow an efficient and convenient formulation of DAE models for dynamic optimization. For this task, we are building on two sets of international collaborations, and are leveraging work done with existing and emerging modeling concepts.

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 2000 with a Visual Basic user interface and with a heavy integration of graphical, simulation and automatic differentiation tools, this software packages was recently updated to incorporate ADOL-C and 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. Future developments of DynoPC will be augmented in collaboration with Prof. Marquardt's group at the Technical University at Aachen (RWTH). Here we are incorporating ESO interfaces, developed by the gProms group that are compliant with recently developed CAPE-Open protocols. This will lead to an interface that will be compatible with a number of existing process models and modeling environments.

Second, we are interfacing and benchmarking our algorithms to other popular modeling enviroments. In collaboration with Prof. Tsatsaronis at the Technical University of Berlin, Tobias and Yuen are incorporating the IPOPT algorithm within OCOMA, 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 plan to exploit the benefits of a MATLAB interface for dynamic optimization. Our future work will enhance the formulation and algorithmic capabilities of MATLAB-based packages like OCOMA and to combine them with our efforts in the development of DynoPC.

Finally, Yi-dong is extending the capabilities of DynoPC to consider parameter estimation and statistical inference for dynamic process models. Dr. Masaru Noda, a visitor from Japan will be working with Yi-dong on optimization applications for fuel cells. Also, Prof. Ricardo Perez is exploring the use of dynamic optimization for biological systems.

Optimization of Pressure Swing Adsorption Systems

Student: **Ling Jiang (Ph.D. started Fall, 1999)**
Researcher: **Daeho Ko (Yonsei University, Korea)**
Industrial Participation: **Grant Fox and Ken Anselmo (Air Products)**

In tandem with the above project, we are also developing more direct sequential strategies for the solution of dynamic optimization problems. These approaches are better known and have seen a lot of previous development. An important 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 does 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.

To take advantage of these algorithms, we have started an NSF/GOALI initiative with Air Products for the optimization of Pressure Swing Adsorption (PSA) systems. For this approach we intend to exploit 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 is 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.*

Daeho Ko recently joined the group and is developing modeling and optimization strategies for PSA units that separate CO2 from flue gases. This is part of a major effort funded by the Department of Energy on CO2 sequestration. Currently, he has developed PSA models in gProms and is working closely with experimental researchers at NETL to combine design strategies with the development of new sorbents. In addition, economic and optimization studies are under way to demonstrate the viability of this approach for CO2 capture.

Synthesis of Reactor Networks for Waste Minimization

Students: **William Rooney (Ph.D. completed April, 2001)**
Visitor: **Shehzaad Kauchali (University of Witwatersrand, returned April 2001)**

Synthesis of optimal reactor networks directly affects all downstream activities and has important implications on separation sequences, energy management and integration and waste minimization. Our previous work dealt with application of geometric principles for defining an attainable region for the reacting system. Here, many literature examples were solved in a simple manner with much better solutions than reported previously. This approach readily deals with arbitrary kinetics and extends naturally to general nonisothermal systems. In general, our approach requires the optimization of Differential-Algebraic systems, but these are not particularly difficult because of our collocation based formulations. An additional advantage to this approach is that it has been integrated within a process flowsheet model so that targeting can be performed for the reactor, with consideration of other aspects of the process, such as heat integration and separation systems.

In particular, our research extended attainable region concepts to more complete MINLP formulations that overcome some of the deficiencies in previous optimization formulations. This has led to a simple superstructure that also incorporates the properties of differential sidestream reactors (DSRs) with optimized sidestreams, which can become important for higher dimensional representations. This approach achieves results that are as good or better than previous studies and overcomes many of the obstacles observed with these studies. To continue this work, we have interacted heavily with Prof. Glasser's group at the University of Witwatersrand. In particular, Brendon Hausberger and Shehzaad Kauchali visited with us over the past two years to develop methods for the construction of attainable regions for reactor networks. In particular, we have been developing prototype concepts for algorithmic generation of

attainable regions using large linear programming formulations. Preliminary results show that this approach is quite encouraging - and can be generalized to a number of multi-dimensional problems.

Moreover, Bill has recently completed his PhD and has joined Air Products. In his thesis, he developed a framework to assess the design of reactor networks with uncertain kinetic and process parameters. This approach incorporates joint confidence regions obtained from experimental data within the reactor design problem as well as other process problems. Use of these regions leads to an approach related to flexibility analysis with some additional structure that can be exploited for efficiency. This approach leads to a multiperiod formulation with additional feasibility tests and has also been extended to uncertainty associated with reactor networks. Here the multiperiod approach employs both AR concepts to generate bounds as well as solution of the MINLP superstructures to develop excellent candidate solutions. Bill has also refined this approach to deal with nonlinear confidence regions. While these are more difficult to generate, especially for larger problems, the confidence regions can be significantly different than for linear models and their impact of robust designs can also be quite different. Bill has developed a number of examples that illustrate this difference.

Finally, in his thesis Bill has considered more detailed approaches to uncertainty. Here we distinguish between uncertainties due to process variability and uncertainties due to a lack of adequate knowledge of the process model. In the former case, control variables can be used to compensate for the variability, especially if these can be measured in a feedforward sense. In the latter case, one needs to develop a robust design that can accommodate all of the uncertainties of the process model. In an actual design application we will generally have both types and here the flexibility analysis becomes more complicated. Bill developed strategies that deal with both types of these uncertainties in a flexibility framework. To solve problems of this type we have also applied constraint aggregation strategies for the flexibility analysis.

Data Reconciliation for Steady State and Dynamic Processes

Students: Nikhil Arora (Ph.D. started January, 1999)

Currently, Nikhil is extending data reconciliation and parameter estimation strategies to both steady state and dynamic processes. He is applying statistical tools to determine steady state conditions, classify measurements and observed model variables, detect data outliers and estimate model parameters. In particular, Nikhil is investigating more general classes of M-estimators for gross error detection within a simultaneous optimization framework. In particular, Nikhil will apply 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.

Following up on our previous work, Nikhil has investigated the Fair function along with a number of redescending functions by Hampl and others. These approaches have the advantage of providing simultaneous outlier detection while at the same time yielding less biased estimates of the reconciled data. Nikhil has benchmarked a number of M-estimators on several literature examples. Preliminary results show that the power (recognition of outliers) is as good or better than with more expensive approaches and that the detection of false positives is also largely avoided. Moreover, this approach has been compared with more expensive combinatorial strategies that apply mixed integer programming. Using the Akaike Information Criterion (AIC) interesting parallels can be derived between robust statistics and the MIP approaches. Moreover, the AIC can be used to tune the parameters in the M-estimator. A paper that describes this approach along with a comprehensive case study for data reconciliation is listed below.

Nikhil is currently developing specialized algorithms that deal more efficiently and reliably with these problem classes. In particular, he is applying bounded trust region strategies to deal with problems that are overparametrized and likely to have nonunique solutions. Preliminary results have shown that these approaches are more reliable 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.

Ignacio Grossmann's Group

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: *Comparative study between MINLP and GDP models for distillation design*

Students: **Mariana Barttfeld (PhD INGAR), Jennifer Jackson [Ph.D. , started Jan 99]**
Collaborators: **Jose Caballero, Juan Reyes [Asistant Profs., Univ. Alicante]**

This project deals with a modeling framework for separation systems based on the State-Task Network (STN) and State Equipment Network (SEN) representations. These models are formulated with generalized disjunctive programming (GDP) models that explicitly handle discrete and continuous variables. The intent is to develop rigorous optimization procedures that do not rely on continuous approximations, which unavoidably introduce complex nonconvexities, and hence are prone to failures and to producing poor solutions. For the reactive distillation columns, a major aim of this work is to develop tray by tray models for synthesis. With the arrival of Mariana Barttfeld from Argentina, the project is currently performing an extensive comparison study of MINLP and GDP models. Both Juan Reyes and Jose Caballero are working in Spain in extending the liquid-liquid extraction model, as well as the synthesis of thermally integrated columns. Below we summarize the state of the project:

Mariana Barttfeld
Mariana has started her work in our group by performing a comprehensive comparison between MINLP and GDP models for optimal design of distillation columns in which tray-by-tray models are used. For the MINLP models she has considered superstructures in which, (a) the feed is fixed and the reflux and reboil returns to a number of potential trays, (b) the reboil is fixed and feed is introduced at all potential trays and the reflux returns to a number of potential trays, (c) like case (b) except the role of reflux and reboil is exchanged. For the GDP model she has considered both the case of fixed reflux, feed and reboiler trays, and all other as conditional trays, and the case where the feed is introduced to all the potential trays. The MINLP and GDP models Mariana has coupled with initialization schemes that she has developed at INGAR in Argentina. These models are thermodynamic in nature, and usually assume that all the potential trays are present at the final solution. While the work is still in progress, the preliminary results suggest, greatly improved robustness of the MINLP and GDP models. As an example, the MINLP of a 50 tray column (ternary ideal; 4149 variables, 3358 equations) took 4.2 minutes vs. 1.2 min with the initialization. More importantly, the no initialization was trapped in a suboptimal solution with 27 trays, while the one with initialization obtained a better design with only 14 trays. Second, the GDP model is often much faster and reliable than the MINLP model. In the previous example starting with 60 trays the GDP method converged in only 16.5 secs. And finally, the MINLP superstructure that seems to work the best for the MINLP is (b), and the second type for the GDP model. We expect to have these results reported in a paper for our next newsletter. The next step that Mariana is undertaking is the application of these models to azeotropic distillation.

Jennifer Jackson: Reactive Distillation
This project is currently on hold. Jennifer assumed that in a reactive distillation column one or several feeds of reactants are given, as well as the stoichiometry and kinetics of the reaction that is assumed to occur in the liquid phase. The major decisions are selecting number of trays, the trays where reaction takes place, and the number and location of feed trays. All trays in the column are treated as conditional, except the condenser and reboiler. Both kinetic reaction and phase equilibrium make take place, or else that no mass exchange takes place in the conditional trays. The possibility of multiple feedtrays is also considered. Jennifer developed a nonlinear disjunctive programming model, which she solved with a variation of the logic-based outer-approximation method of Metin Turkay. Jennifer has solved two problems. One is the methatesis reaction in which 2-pentene reacts to give 2-butene and 3-hexeneusing ideal thermodynamics and second order kinetics. For a potential column with up to 25 trays, Jennifer obtained a design with 21 trays, with the feed of pentene distributed over 5 trays. The reactive zone of the column is given by trays 1-

18 (1 is the lowest tray). Jennifer was able to show that restricting the feed into one tray, a suboptimal solution is obtained which is about $15,000/yr more expensive. In terms of computation, the problem size involved 25 discrete variables, 731 continuous variables and 730 constraints, as well as 25 disjunctions, and was solved in 3 major iterations in 168 secs on a Pentium III machine..

Juan Reyes: Liquid-Liquid extraction
Juan Reyes is currently exploring the use of global optimization techniques for the optimization of superstructures for liquid-liquid extraction systems. The major alternatives embedded in that superstructure are the selection of number of stages, location of intermediate feeds and extractions, splits and selection of solvents. Juan generalized the superstructure for the case of multiple feeds of the liquid that is to be extracted, and formulated the model as a disjunctive programming problem, also using the concept of conditional stages. Initially the idea is to try to implement some of the ideas developed by Sangbum Lee for global optimization.

Jose Caballero: Thermally linked columns.
Jose is currently looking at the issue of systematically generating all the configurations for thermally integrated distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. Jose has developed a set of logic propositions that can serve as constraints in an MILP or MINLP model to define the search space for thermally integrated columns.

Operational Planning and Retrofit Design in Process Networks

Students: **Jennifer Jackson [Ph.D., started Jan 99]**
New Development: *Multiperiod Planning model for Multisites*

Jennifer's project has been concerned with developing high level optimization models for process modifications. Her work was then redirected to a project with Dow, dealing with multiperiod optimization of a network of polymer plants, which is currently being extended to multisite optimization..

The initial problem that Jennifer considered is the one in which an existing network of processes is given, and for which process modifications such as improvement of yield, increase of capacity, or reduction of energy consumption and/or waste generation are considered over a period of several years. The problem consists in identifying retrofit projects for those processes that will yield a maximum improvement in the Net Present Value. Jennifer developed a generic linear model for processes in which the various types of modifications can be incorporated. The problem is modeled as a multiperiod disjunctive programming problem that can be reformulated as an MILP. Disjunctions are used to select from among the several alternatives for process modifications. Jennifer had tested these ideas on a network with 5 processes that include processes for producing acetaldehyde, acrylonitrile, acetone, phenol and cumene, and obtained very good results compared to solving a conventional MILP problem. Jennifer also looked at the question on how to rank the retrofit projects in decreasing order of potential economic impact without considering the more detailed multiperiod operation. The motivation for performing the ranking is to identify the most promising alternatives for which a more detailed study is performed and included in the multiperiod model described above.

Jennifer has essentially completed joint project with Dow. The problem considered is the multiperiod optimization of a network of polymer plants. In that problem a horizon of one year is considered, and the goal is to determine the production of a given number of different polymers so as to maximize profit. An important feature of this problem is that nonlinear empirical models available for each of the plants. Jennifer developed a multiperiod NLP that considers the assignment of products to be produced at each plant. The effect of inventories is taken into account. Transitions are not an issue since extensive use of blending of various products is performed. Jennifer demonstrated on this project the advantages of GAMS over Excel, which was initially used to address monthly productions. Jennifer's model was tested with plant data resulting in good agreement. Also, with the help of Gabriela Garcia the model has been implemented on the web, in which the automatic interface with GAMS takes place.

Jennifer has recently started to extend the above model to a supply chain optimization problem involving multiple sites of production and multiple markets in which the transportation of products is considered. While the model is conceptually similar to the single site case, the major difficulty becomes the large size of the problem, which makes it very difficult and expensive to directly apply NLP algorithms for the solution. In order to address this issue, Jennifer has explored the use of Lagrangian relaxation, in which the material flows between plants and markets are dualized, which in turn allows the suboptimization of each system for fixed multipliers to produce upper bounds for the profit. These multipliers are updated with a common subgradient optimization procedure. Aside from duality gaps, a difficulty that arises is the generation of feasible solutions to predict lower bounds. To overcome this problem Jennifer has used relaxation and readjustment of the mass balances for the markets that are linear. Preliminary results on a problem involving 3 production sites, 3 markets, 8 time periods (months), and which led to an NLP with 13377variables and 11398 constraints, the Lagrangian decomposition managed to get within 9% of the optimum with 20% of the computation time of the NLP (550 sec vs. 2350 sec).

Algorithms for Nonlinear Disjunctive Programming

Students:	**Sangbum Lee [Ph.D., started Jan 98]**
Research fellow:	**Aldo Vecchietti [Ph.D., completed Aug 2000]**
New Development:	*Global optimization of GDP with bilinear equations.*
	Superstructure optimization of olefins plant.

Sangbum Lee: Nonlinear GDP

The objective of Sangbum's project is to develop solution methods for nonlinear generalized disjunctive programs involving multiple terms in the disjunctions that are given in the form:

$$\text{Min} \quad Z = \sum\sum c_{ik} + f(x)$$

$$\text{st} \quad g(x) \quad 0 \qquad \text{(GDP)}$$

$$\bigvee_{i \hat{I} D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(x) \le 0 \\ c_{ik} = \gamma_{ik} \end{bmatrix} \qquad k \hat{I} SD$$

$$W(Y) = True$$

$$x \hat{I} R^n, c \hat{I} R^m, Y \hat{I} \{true, false\}^m$$

Sangbum considered first the case when the nonlinear functions are convex. He showed that a convex NLP relaxation model can be derived that is based on considering the convex hull for nonlinear convex inequalities. This NLP has the property that it gives stronger lower bounds than the ones that are obtained with the corresponding MINLP with "big-M" constraints. This NLP relaxation can be used in two major ways: (a) to reformulate the above GDP as an MINLP, which can then be solved with existing methods, (b) to develop a specialized branch and bound method that makes use of the new NLP relaxation by branching on the terms of the disjunctions rather than on the 0-1 variables. The reformulation and the branch and bound algorithm have been applied to various GDP problems, demonstrating that significantly improved lower bounds were obtained in most problems.

Sangbum then moved to develop a global optimization algorithm for solving Generalized Disjunctive Programming problems involving nonconvexities in the form of bilinear, linear fractional terms and separable concave functions. The main idea behind the proposed method is to perform a branch and bound search with the convex NLP relaxation that results from replacing the nonconvex terms with convex

envelopes, and apply the convex hull over the disjunctions that have not been selected. When feasible discrete solutions are found in the tree, the resulting reduced NLP subproblem is solved with a spatial branch and bound method for global optimization. Sangbum used a variation of Juan Zamora's and Ignacio Quesada's algorithms for this purpose. Sangbum applied this algorithm to several examples that include small separation problems, a heat exchanger network, pooling and blending with fixed charges, and synthesis of batch processes in which the major problem consists in deciding what tasks are assigned to which equipment, with the possibility of merging tasks to reduce the number of equipment. For a set of 8 problems the proposed global optimization method found improved solutions in half of the problems when compared to solutions obtained with DICOPT. While the CPU times are typically one order of magnitude larger, the requirements are still reasonable considering that one obtains rigorous guarantees of globality.

Based on the work on global optimization described above, Sangbum has addressed the optimization of process networks when bilinear equations are involved in the disjunctions. One interesting issue that also arises here is whether the use of total flows and compositions is better than using individual flows. The basic idea in Sangbum's method is to formulate the problem initially in terms of flows and compositions, and then apply McCormick underestimators together with reformulation-liunearization, which leads to a relaxation of the GDP. By applying the convex hull to each disjunction, the lower bounding LP or NLP is obtained that is used within the two level branch and bound method for global optimization. Sangbum has applied this method to process network problems with discrete variables related to pooling and blending, wastewater treatment and water-usage networks. Interestingly enough in each of the cases improved solutions were found over DICOPT's use in the MINLP version. The computing times varied between 37 and 230 secs. Sangbum is in the process of completing the manuscript related to this work.

In yet another part of this project, Sangbum looked recently with Aldo Vecchietti at the characterization of disjunctions, and the impact of relaxations for the big-M and convex hull relaxations. Disjunctionscan be divided between proper and improper. As a simple example consider the disjunction $R_1 \vee R_2$. If $R_1 \subseteq R_2$. the disjunction is said to be *improper*, because one set contains the other. If this does not hold, the disjunction is said to be proper. If we analyze the disjunctions in the space of x it is clear that the convex hull reduces to the largest region containing the other terms, and therefore there would be apparently no incentive to use the convex hull reformulation. Numerical examples, however, showed that the convex hull did yield improvements in this case. This result puzzled us for quite some time, but fortunately, Sangbum solved the puzzle. It turns out that while the convex hull is indeed identical than the larger term of an improper set in the space of continuous variables, it is not true in the space of discrete and continuous variables. Sangbum has a small geometrical example that illustrates this property very clear. We enclose a copy of this paper, which also includes a cutting plane algorithm as an alternative to using the explicit equations of the convex hull.

In collaboration with Michael Domach, a faculty from Chemical Engineering in bioengineering, Sangbum was involved in the problem of finding all the alternate solutions of an LP related to a metabolic network. He developed an MILP formulation that can be applied to LPs with variables that are unrestricted in sign, and that may exhibit degenerate solutions. The proposed method was applied to the LP of a metabolic network involving about 50 variables and constraints, and with up to 30 alternate optima. This work has now been implemented by a student from Mike Domach, and is used as a screening tool for conducting NMR experiments.

Finally, if it not were enough, Sangbum has initiated a special project in collaboration with BP that deals with the superstructure optimization of an olefins plant, and in which we anticipate being able to use Sangbum's methods. Sangbum is at the initial stages of developing the superstructure and putting together simplified models for this problem.

Aldo Vecchietti: LOGMIP and modeling issues

The project by Sangbum is being complemented by Dr. Aldo Vecchietti from INGAR in Argentina. The main thrust of the work by Aldo has been the developments of LOGMIP, as well as the analysis of alternative models for disjunctive programming, which was described above. Aldo is also developing a PC version of the new 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) 0 => f(x) 0) can be systematically converted in the form of disjunctions. As for the propositional logic, we have decided to develop special constructs such as ASSIGN, ATLEAST, ATMOST, IMPLIES, etc. to facilitate the specification of logic conditions. For the general case, the propositional logic can expressed in symbolic form, and a previous PROLOG program developed by Michelle Tourn is being used as a basis. 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.

Aldo is currently completing the implementation of the convex hull relaxation for linear problems. He has implemented both the regular and the embedded disjunctions in the IDE verson of GAMS. He is also testing the prototype on several example problems.

Optimal Design and Planning of Oilfield Infrastructures under Uncertainty

Students: **Vikas Goel (Ph.D. started January 2001)**
New Developments: *Preliminary results for oilfields with uncertain size and quality*

Vikas has been continuing the efforts of Sarette in the area of oilfield planning, with the major focus of the work being the handling of uncertainties. He is using as a basis two of the previous deterministic models by Sarette. One is for the case when the selection of production and well platforms is performed, together with the location and schedule for drilling wells. The nonlinearities in this multiperiod problem arise for the predicting the pressure in the reservoirs and the corresponding cumulative production flow of gas and oil. For this case Sarette developed a bilevel decomposition strategy that involves solving nonlinear disjunctive problems at each level. The other model by Sarette addresses a different version of the problem that deals with gas fields and in which we do not consider the drilling of wells, but we consider possible interconnections between wells platforms, as well as complex objective functions that include royalties, taxes and tariffs. This case was solved through a Lagrangian decomposition method.

The two biggest sources of uncertainty that Vikas intends to address in his project are the price of oil, and the productivity of the wells. Vikas has started by considering the latter. As an initial step he has considered discrete distribution functions for the well productivities in a gas oilfield in which the configuration of well platforms is given. Furthermore, it is assumed that some of the platforms are already in operation, while the rest are not. The problem then consists in deciding which well platforms to install and when to drill their corresponding wells. One approach for handling this case is to consider a two-stage programming strategy in which the selection of well platform and their capacities are considered as stage-1 variables, while the production levels and flows are considered in a second stage. Using this strategy the problem can be transformed into a multiperiod optimization problem. The difficulty however, is that the number of scenarios that must be considered for each time period can be very high, leading to a very large scale MINLP problem. As an example a problem with 10 fields involves over one million scenarios. What Vikas has been exploring is a decomposition scheme that exploits the fact that each well platform has only "major" operarting modes corresponding to the discrete realizations corresponding to the well associated with that platform.

He has applied these ideas to the gas oilfield problem by Sarette. The uncertainties that he has considered are the size of the field (total recoverable gas) and its quality (maximum rate of recovery). The proposed method by Vikas relies on a Lagrangian decomposition scheme for aggregating the multipliers connecting the production and well platforms, so that the net result is that each well platform must be optimized only for its "major" operating modes, which drastically reduces dimensionality of the multiperiod problem. Due to the duality gap, convergence is stopped after a prespecified number of iterations (typiically 10-20). Vikas applied this scheme to a problem involving 5 fields (2 uncertain), which gives rise to 16 scenarios since there are two discrete probabilities for each parameter (size, quality in each field). Using a full space method (about 10,000 constraints) required more than twice the time (474 sec vs 196 secs). For the case of

3 discrete probabilities (81 scenarios), the proposed method was more than four times faster (3,500 sec vs 15,500 sec). Vikas also showed that the predicted well platform capacities are significantly different when compared with the ones predicted by the deterministic model. The limitation of this method is that the subproblem that remains with the dimensionality of the total number of scenarios, is the optimization of the production platform. Vikas is currently exploring several aggregation alternatives for reducing the size of thius subproblem.

Scheduling and Planning of Hydrogen Pipelines

Student: **Susara van den Heever (Ph.D. started January 1997-completed April 2001)**
Postdoctoral fellow: **Iiro Harjunkoski (started September 1999]**

In the last part of her Ph.D. work Sarette addressed an interesting problem of hydrogen supply pipelines in collaboration with Dr. Mark Daichendt from Air Products. The problem is the one in which a set of production plants for hydrogen is given, as well as several supply points in a pipeline that connects sources and destinations. Given a number of time periods with forecasts for demand the problem consists of determining the level of operation at each plant (e.g. which compressors to operate), as well as the policy for storing hydrogen in the pipeline through manipulations of the pressure. Sarette developed a planning and a scheduling model, in which the planning model is concerned with determining the production targets in each plant, and the scheduling model the detailed delivery of hydrogen to each destination point. She used a rolling horizon strategy in which the planning model is solved successively with one period of the scheduling model. Since the planning model can become quite large, and represents the bottleneck in the rolling horizon, Sarette developed a Lagrangean decomposition scheme that proved to be very successful. For instance, in a problem with 14 time periods the full space MINLP could not be solved within 10 hours, whereas the proposed decomposition method required only of the order of 20 minutes. Another major issue that Sarette had to struggle in this model is the handling of nondifferentiabilities that are due to the equations that involve absolute values, and sign and max operators. Iiro Harjunkoski continued the project by first revisiting different options for handling the difficult nonlinearities that give rise to non-differentiabilities. Numerical results, however, showed that the models that Sarette developed were the ones that led to the best computational results. Gabriela Garcia implemented Sarette's model in an interface to facilitate its use.

Scheduling of Batch and Continuous Multiproduct Plants

Postdoctoral fellow: **Iiro Harjunkoski (started September 1999]**
New Development *Completion of hybrid models for multistage batch plants*

Iiro joined ABB in Germany in September. We briefly summarize here his work. One of his projects was the integration of CP (Constraint Programming) and MILP. Initially, Iiro applied the decomposition idea to the trim loss problem, which is a MINLP problem where wide raw paper reels are to be cut into narrower product reels by minimizing the waste, as well as, some other production parameters such as the number of different patterns needed. The approach that Iiro developed was to linearize the MINLP by introducing new variables that correspond to products of discrete and continuous variables. This MILP corresponds to a relaxation that yields a lower bound, and often yields very good approximations of the original problem. At that stage the problem of finding a feasible solution with the original nonlinear integer constraints is reformulated as a CP problem with a fixed value of the objective. If no feasible solution is found, the value of the objective is increased and the CLP is resolved until a feasible solution is found. This approach proved to be very efficient compared to the direct solution of the MINLP.

Iiro developed a similar strategy for the short-term multistage batch plant scheduling problem that Jose Pinto studied in his Ph.D. work, and is implemented in the STBS interface. The only difference is that Iiro uses as the objective to minimize the cost of assignments to orders to machines, instead of minimizing tardiness. The idea in Iiro's work has been to partition the assignment and sequencing decisions by solving a relaxed MILP for the former, and a CP problem for the latter in the spirit of Vipul's hybrid strategy. Iiro, however, also tried to use an MILP for the sequencing phase, as this has the advantage that the same solver

can be used. Generating rigorous tight cuts for the MILP in this problem, however, has turned out to be surprisingly difficult. Iiro found new cuts that can be derived from a graph representation of the schedule. The basic idea consists in tracing back all the paths that are initiated from tardy jobs in the last stage to the first stage going through bottleneck assignments. This procedure may generate in fact more than one cut. The numerical results essentially have shown that it is generally advantageous to use CP for the sequencing part, although the times for the MILP were by no means excessive. The other result was that came out is that as opposed to the case of single stage plants, which had been addressed by Vipul Jain, the case of multiple stages did not always show the consistent large gains that had been achieved for single stage systems. Nevertheless, in one of the largest problem (3 stages, 8 machines, 12 jobs), the MILP (CPLEX) required 2767 secs, and the CP (ILOG) required 712 secs. The hybrid strategy required in contrast only 14 secs. A copy of the paper describing this work is enclosed

Regarding the collaboration with Kvaerner, Iiro left his program for the scheduling of a steel plant. Iiro developed an effective decomposition approach that consists of the following major steps: (a) presorting of orders into product families, (b) disaggregation into groups that are to be scheduled independently, (c) flowshop scheduling of each group, (d) overall scheduling for joining the groups, (e) final refinement. Steps (b), (c) and (d) are performed with MILP models, while the last step is solved with an LP. This decomposition has the advantage of allowing the solution of large problems. The disadvantage is that it is a heuristic. However, Iiro was fortunately able to find an expression for computing a *lower bound* to the makespan, and found that in the examples given too us the maximum deviations from the global optimum were a maximum of 1 to 3%. The proposed approach has been applied to several one-week production scheduling problems (80-100 orders). The total CPU-times required with XPRESS ranged between 7 and 170 minutes. More importantly, the schedules found had makespan of the order of 5 days and 8 to 20 hours, which compared to the maximum of 7 days represents savings in production time between 17 and 24%.

Uncertainty in the Scheduling of Batch Processes

New student: Jayanth Balasubramanian [Ph.D. started November 1998]
New: New approach based on interval arithmetic, fuzzy sets for uncertain processing times

Jayanth's project deals with batch scheduling problems in which the uncertainties considered are processing times. The conceptual problem is to find a schedule that minimizes the expected completion time. Jayanth has concentrated his work on batch flowshop and parallel line scheduling problems, as well as scheduling for new product development. In all cases the major source of uncertainty considered are the duration times.

In his initial work Jayanth developed a branch and bound procedure for flowshops with zero wait policy in which the key ideas are the following. First, for a fixed sequence the analytical expression that was proposed by Karimi is used to simplify computing the expected completion time. The idea is then to exploit the property that the expected value of a sum is the sum of expected values (assuming independence). This property reduces to few hundreds the evaluations for the expected completion time given a state space with trillions of states of discrete probabilities. 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, he replaces by expected values, which guarantees their lower bound properties. In the implementation that Jayanth has done in Java he was able to solve problems with up to 9 products and 3 stages with $7x10^{12}$ scenarios. That particular problem, which cannot even be generated for a conventional multiperiod equivalent, required 1600 secs for solving the problem to optimality. Smaller problems required considerably less time. For instance a problem with 5 products and 3 stages with $4.7x10^{11}$ scenarios required only 3.5 secs. Jayanth has also to 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.

Jaynath has also addressed the problem of parallel units with uncertain processing times, in which he has been able to exploit similar lower bounding properties. In this case the evaluation of the expected completion time for a fixed schedule can be performed quite effectively. However, the optimization with branch and bound is much harder. Therefore, Jayanth has explored the application of a genetic algorithm to optimize the schedule. Using this approach, he obtained generally good results.

Motivated by the need to develop computationally efficient methods for optimizing schedules with uncertain tasks, Jayanth has developed an 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. In order to better understand the relationship of this approach with probabilistic methods, Jayanth developed general guidelines and a specific example, which shows the following. The probabilistic approach requires multiple integrals, while the new approach only involves single dimensional integrals. To extend this approach to optimization there are two options. One is to use MILP, which can be done without great difficulty since the dimensionality of the problem does not increase exponentially with the size of the problem. The other approach is to use a direct search method (e.g. tabu search, genetic algorithm). A major advantage of the method developed by Jayanth is that it can be adapted without great difficulty to a variety of scheduling problems. Jayanth has applied this to scheduling problems for flowshops and for new product development. In the case of flowshops h 12 products and 4 stages (48 uncertain times). As a comparison with the probabilistic approach in a problem with 8 products and 4 stages, Jayanth's procedure required about 28 sec while the probabilistic approach required 4 hours! Jaynath has also solved new product with up to 65 tests, which is a sanitized version of a problem by DowAgro Sciences. The resulting MILP involved 4061 binaries, 8794 continuous variables and 267,912 constraints, and was solved in about 45 minutes with CPLEX. Jayanth is currently writing a manuscript on this work.

Integration of Product Testing and Planning of Batch Manufacturing Facilities

Student: **Christos Maravelias (Ph.D. started January 2000)**
New Developments: *Computational experiments for resource constrained scheduling*

The research project of Christos 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 as follows. Given is a time horizon 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 then 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.

Based on the continuous time model by Craig Schmidt for scheduling for new product development and its extension by Vipul Jain for resource constraints, and the discrete time linear model for flexible process networks by Norton, Christos was able to integrate both models through a novel MILP model. Furthermore, Christos found a tighter representation of the resource constraints compared to Vipul's work. The proposed model is augmented with 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 similar to Sarette's. In Christos' case 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 scheduling problem, Christos has revisited that problem, which Vipul Jain had addressed. Christos has explored a number of alternative solution methods including Lagrangean relaxation, a heuristic decomposition, Benders decomposition and branch and cut. With Lagrangean relaxation he found that one could decompose the problem by products, and very good solutions would be generated within the first few iterations, but the gap of the bounds was quite large. Christos then developed a heuristic decomposition in which the unrestricted scheduling problem was solved first for each product. The binaries for the ordering were then fixed in the original MILP model, in order to find schedules that accounted for resource constraints and possibility of outsourcing. Benders decomposition proved to be more expensive than full space. This produced significant reductions from couple hours, down to 5 to 15 minutes.

The more interesting results were obtained with cuts. Christos found that adding cycle breaking cutting planes would greatly improve the LP relaxation, and that to avoid adding all of them up front, one can add only the ones that are violated in the root node. This means for example in a 65 test problem, that instead of having to add about 90,000 constraints up front, it is sufficient to add about 18,000 that become violated. A closer examination of this approach led to the interesting idea of adding as cutting planes, implied precedences, which in fact can be regarded as logic cuts. For example if A is followed by B, and B followed by C, then A followed by C is an implied precedence. Christos first applied this idea for problems with fixed precedence constraints and obtained excellent results. As an example he found in the larger problem that the time of the MILP could be reduced from 2.5 hours down to only 15 minutes. Christos is now trying to formalize this idea and apply it through logic inference within the branch and bound enumeration procedure.

Supply Chain Dynamics and Control (joint with Erik Ydstie)

Student: **Edgar Perea (Ph.D. started January 1997)**
New development: *MILP model for Model Predictive Control scheme*

This is a joint project with Erik Ydstie in collaboration with Turaj Tahmassebi. from Unilever. The problem that Edgar has addressed is the one of determining the dynamic response of a supply chain to perturbations in the demand, as well as determining optimal levels of inventories and production policies. The two major approaches that Edgar has developedd are a decentralized control approach through simulation, and a simultaneous optimization approach through Model Predictive Control.

The supply chain considered is one that consists of a manufacturing plant, warehouse, distribution center and retail center. The manufacturing plant can produce multiple products. In this supply chain the material and information flows that go in opposing directions are the following: the material flow from the plant to the retail center; the information flows from the retail center to the manufacturing plant in the form of orders. When disturbances occur in the demands at the retail level, there is often an amplification of the orders upstream due to the decentralized decisions made at each point of the of the supply chain. For the decentralized approach, Edgar modeled with tanks the accumulation of material and the accumulation of order at each stage of the supply chain. Also, he postulated delivery rates for the materials as well as control laws for the decisions at each point of the supply chain. For the manufacturing plant a similar control law was postulated which in effect corresponds to a heuristic scheduling method. The dynamic simulation of this model gives rise to a hybrid system since discrete decisions are involved in terms of switching manufacturing to different products in the plant, and in terms of managing the inventory levels at each stage. Edgar was able to model the problem in Matlab and solve it using Signalflow. He analyzed with different control laws (e.g. feedback based on set point for inventory levels) how closely the supply chain

was able to track the demand of customers, as well as determining the dynamic response in the inventory levels. He has also verified the upstream amplification of signals that are experienced in supply chains (Forrester effect). For the selection of gains Edgar concluded that they can be selected based on physical grounds. On the delivery rates he has found that the responses tend to be rather sensitive, and that accounting for inventories does help significantly to dampen the responses.

For the simultaneous optimization of the dynamic model for the supply chain, Edgar has adopted a Model Predictive Control approach using a rolling horizon. The optimization is performed simultaneously at the level of scheduling in the manufacturing plant, and at the global level for coordinating inventory in all stages of the supply chain and providing the parameters of the control laws. Initially Edgar tried a "flat" simultaneous multiperiod MINLP model in which the dynamic DAE model was converted in algebraic form through collocation, and optimized together with the schedule and inventory levels. Since this model proved to be a very hard problem to solve, Edgar used a discrete time approximation for the DAE system that allowed him to formulate the problem as a large scale MILP. Since the control laws for the distribution channels and the manufacturing sites are found simultaneously, the model captures all the interactions within the system and can find better solutions. By using profits or infinite norm for customer satisfaction level as the objective function, the system is simplified to a sequential solution of MILPs over a rolling horizon. Edgar has applied the MPC approach to a supply chain consisting of 3 plants producing 3 products, 3 plant warehouses, 4 distribution centers, 10 retailers and 10 demand regions. He considered a rolling horizon of 2 weeks with 2 hour intervals, and with a demand that follows a periodic behavior. He compared the results of this integrated approach versus the cases when only the schedule or only the distribution was optimized. In both cases, Edgar found that the integrated approach was able to yield higher profits by significantly reducing the inventories through better coordination between manufacturing and distribution. Edgar is currently writing a paper based on this work.

Optimal Multiperiod Planning for Catalyst Replacement

Research Assistants: **Martin Houze (started January 2001)**

This project is being conducted by Martin Houze as part of a joint collaboration with Totalfinaelf through Nikola Juhasz. The problem is as follows. Given is a continuous polymer plant 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 planning 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, Martin developed a semi-empirical model that provides reasonable fit with the plant data. He has used that model as a basis to develop a multiperiod MINLP model for deciding the optimal catalysts replacement, and operating conditions. The model has evolved to a point where its solution is quite reliable. The model has been applied to problems between 2 and 4 years. Also, despite the presence of nonconvexities, Martin has found that DICOPT has almost always found what appears to be the global optimum. The difficulty has to do more with the trend of the model to predict higher catalysts temperatures, which will age faster the catalyst. Martin is trying to correct this with an improved model for the deactivation of the catalyst. .

Software for MINLP Optimization in Design and Scheduling

Research Assistants: **Gabriela Garcia (started March 2000)**
Collaborators: **Dr. Zdravko Kravanja, Univ. Maribor, Slovenia**
New Developments: *Web interface of WATER*

Gabriela has continued developing a framework for migrating the interfaces to the web. The motivation is first to provide easier access to the users. 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. They would all be running from a server at CMU. This project has also been inspired by the joint collaboration with Dow in which the final implementation will be performed on a web-intranet system.

The first interface that Gabriela has implemented on the web is WATER, which is based on the work of Berta Galan for the design and synthesis of water treatment systems. This interface determines the optimal configuration of m treatment units given n streams that need to have several contaminants removed. Gabriela has also been porting from UNIX to the PC, the interface PRODEV that deals with scheduling model for new product development by Craig Schmidt. 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:

SYNHEAT MINLP synthesis heat exchanger networks *(Yee)*
Also includes transshipment model for targeting *(Papoulias)*

STEAM MINLP Model for the synthesis of combined cycles for utility plants (Bruno)
Model includes correlations for steam, efficiencies and cost data

GLOBESEP Global NLP optimization for synthesis of separation networks and single feed/mixed products *(Quesada)*

WATER Global NLP Model for synthesis of wastewater treatment configuration *(Galan)*

EXTRACTOR Disjunctive MINLP for synthesis of liquid-liquid extraction systems *(Reyes)*

Batch design:

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

BATCHMPC MILP model for multiproduct batch plants
mixed-product campaigns *(Birewar, Voudouris)*

Scheduling:

PARALLEL MINLP continuous multiproduct scheduling on parallel lines
Features feasibility preanalysis *(Sahinidis)*

MULTISTAGE MINLP continuous multiproduct in multistage plants *(Pinto)*

CYCLE LP/MILP aggregate flowshop scheduling (cycle time/makespan)
Includes loop tracing algorithm *(Birewar)*

STBS MILP short term multistage scheduling *(Pinto, Bolio)*

CRUDEOIL MILP model for refinery scheduling *(Lee, Pinto)*

DECAY MINLP model for scheduling of clean-up of parallel furnaces *(Jain)*

UTILPLAN MILPmultiperiod model for utility plants *(Iyer)*

PRODEV MILP model for scheduling of tests in new product development *(Schmidt, Najimas)*

Planning:

PLANNER MILP multiperiod model for capacity expansion in process networks
(conventional and lot sizing model) *(Sahinidis, Norton)*

MULTISITE MILP model for planning the selection of processes and capacity expansion in different geographical location and accounting for transportation costs *(Turkay)*

GREENPLAN Bi-criterion MILP model for selection of processes that maximize the net present value and minimize toxicity *(Drabbant)*

NETCHAIN Multiperiod MILPfor supply chain optimization of multisite facilities with flexible processes, intermittent deliveries, changeovers and inventories *(Bok/Iyer)*

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 difference 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?

PROGRESS

Continuing to explore his decomposition strategy for reactive separation design, Warren has concentrated on working out the feasible region in a single counter current section with simultaneous reaction and separation. For a given amount of overall chemical reaction, there are two possible reachability bounds depending on the local VLE behavior around the non-reactive pinch point. Although the overall amount of reaction is fixed, Warren's studies have exposed the impact of internal reaction distribution policy. A number of the geometric features previously found only in strongly non-ideal distillation systems -- including fold points, multiple pinch point branches and composition regions separated by bifurcation loci -- have been discovered for reacting system even in the presence of ideal phase behavior. A manuscript demonstrating the insights obtained from generalized difference point and parts of the (still incomplete) analytical techniques developed is included with this newsletter. The new thing here is how regional analysis in composition space may be used to predict feasibility and placement of reactive stages to avoid external recycle in an azeotropic system.

Agent-based, Asynchronous Process Design

Student: John Siirola (PhD, started Jan 2001)

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 available in the form of distributed computer cluster. This work continues that started by Ken Tyner 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:

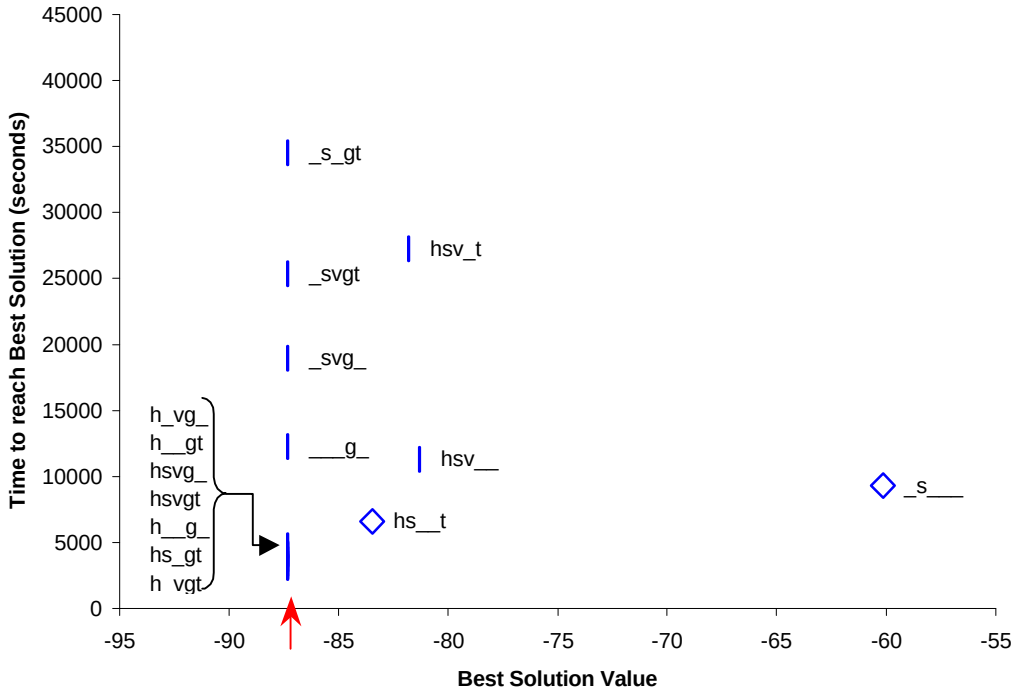
1. The master resource control loop determines the individual agents' access to computing power. With the assumption that the number of possible cases to run is substantially larger than the available resources, selecting a promising agent-pool with sufficient variability becomes a crucial step in solving 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 has set up an example problem on which to demonstrate the effect of agents helping each other to find solutions. The problem is an objective function comprising the sum of a number of sinusoidal functions with differing frequencies and amplitudes. Thus it has many, many local optima. For example for five degrees of freedom, it has 5x10^8 local optima, with five of them being the global optimum. John has created several types of agents. For optimization, he has a gradient-based hill climber implemented in GAMS, a simulated annealer and a genetic algorithms - both in PERL. He also has a "look for places where there is a paucity of points" algorithm. Finally he has an agent that will eliminate points that are in regions where no good points have ever been found. He can activate many copies of each of these algorithms, each with different parameterizations so they will behave differently.



Shown in the figure is the behavior when using different combinations of agents. To find the global optimum (the left most points) in the least time (the lower points) happens only when the system includes combinations of agents. The symbol hs_gt means he used multiple copies of the hill climbing, simulated annealing, genetic and "data trimming" types of agents. Also, only for these same combination of agents are all the local optima routinely found.

He solved a ten degree of freedom problems also, where there are 10^17 local optima, with ten being global. He completed a study in which all different combinations of agents - e.g., only a single version of the simulated annealing algorithm or only the genetic algorithm, or many of the simulated annealing algorithm, or five of this agent with seven of that, and so forth - are set loose on the example problem. Again, only when using combinations of agents does one find the global optimum. Most times the better combinations of agents will find all the global optima.

Current focus has two components:

- efficient formulation of functions with multiple objectives
- strategies for data reduction to perform regional pruning and avoid system atrification.

The upgrade of our Beowulf computer cluster also continues: We now have 32 dual-cpu computing nodes as well as 2 administrative machines on a custom version of RedHat Linux with a scalable infrastructure as well as easy installation and maintenance. The project is funded by NSF and Intel Academic relations. A facility upgrade in Doherty Hall is expected to complete before Christmas and will provide sufficient electrical power and cooling for planned and future expansions.

Microscale Process Design

Students: Anton Pfeiffer (PhD, starting Jan 2001) and Michael Bartovsky (PhD, starting Jan 2001)

Collaborators: Todd Pryzbycien (Biomedical Engineering), Kaigham Gabriel (Electrical & Computer Engineering), Victor Weedn (Biology), Tamal Mukherjee (ECE), Jim Hobugh (ECE) and Qiao Lin (ME)

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,
(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.

A project currently in an exploratory phase is MEMS-based micro-gravimetric sensors which offer the possibility of low-cost detection devices of biomolecules in the ppm. The basic principle consist of a chemically functionalized membrane surface to which only specific proteins will bind. By vibration and subsequent identification of resonance frequencies, the presence of target molecules may be detected with exceptional accuracy. The concept has been demonstrated for macroscopic systems in Todd Pryzbycien's group using a 1-D vibrating quartz crystal. In additional to many practical design questions, system level issues include optimal functionalization of a 2-D surface as well as configuration and operation of detector arrays.

PROGRESS

These projects are just getting off the ground with new PhD students joining officially in January 2001.

A project for electrophoretic separation has been funded by DARPA. The initial goal is to develop "black box" models for calculating the optimal separation resolution and corresponding chip layout based on a user-supplied structure. One of the key aspects is to understand the underlying physics and capture the behaviour in a sufficiently simple model; this is being pursued with collaborators in ECE and ME.

The membrane for use in gravimetric detection has been fabricated and successfully covered with gold in preparation for attaching the relevant ligands to the surface.

Flexible Synthesis of High-Value Products

Student: Murni Ahmad (MSc, started Jan 2000)

BACKGROUND

Co-advised by Todd Przybycien, Murni is working on optimal design and operation of pharmaceutical and biochemical processes. In addition to regulatory constraints imposed on the operation of actual equipment, modeling is further complicated by incomplete knowledge of the biological mechanisms involved and different assessment of time-to-market aspects compared to production of bulk chemicals. A key issue is to capture the economic interactions between efficiently designed processes in new equipment in light of procedural requirements for FDA approval. A problem is that thermodynamic models and parameters are associated with limited validity and large uncertainty. Consequently, individual designs as well as scaleup must be done by a collection of models.

PROGRESS

Murni has reformulated and generalized the thermodynamic models for the binodal 2-phase split as well as protein partition for systems with both polymers and salts. She is currently implementing an optimization framework for two-phase extraction systems in Matlab. She will submit her MSc thesis in December and continue her work as a PhD student.

Gary Powers' Group

Process Risk Assessment Using Symbolic Model Checking
Students: Dan Margolis and Dan Milam

The work by doctoral students Dan Margolis and Dan Milam is focussing on the more rapid generation of models for risk assessment. Symbolic model checking which is used in the checking of VLSI circuits holds a promise for the verification of the correctness of complex chemical process control systems including interlocks, alarms and operating procedures. The current challenge is to describe the chemical processing system with discrete event hybrid models of sufficient validity.

Dan Margolis is working on the operating procedures that describe the logic of how operators and maintenance workers interact with the process. He is building an operating procedure language that can be interpreted into the discrete event language currently used in Symbolic Model Checking. He is also considering how the synthesis of operating procedures could be guided by the Model Checking approach. He is building on the research of Dr. Bob Fusillo and Dr. Tom Teague both of whom worked on the operating procedure synthesis problem. He is currently applying this approach to a computer controlled casting system.

Dan Milam is generating a library of modular models that can be interconnected to generate system models for use by the Symbolic Model Verification program. He is developing methods for the synthesis of discrete event hybrid system models, which are derived from the specifications, which are to be checked on the process. The coverage of these models (do they include 'all' the important behaviors) is being investigated both theoretically and experimentally. Mr. Milam's work is using the research results from Dr. Scott Probst and Dr. Adam Turk. He is currently applying this approach to a computer controlled casting system.

Supot Lertsakulsup is working on a Masters research project for the application of model checking in the safety assessment of off-shore platforms for the production of oil and gas.

Miguel Vescovacci will be working on a Masters project for the development of a model library that will contain models that can be validated by information from international failure databanks and by comparison with simulations and experimental data.

Arthur Westerberg's Group

Life Cycle Analysis with Structured Uncertainty for the Synthesis of Process Flowsheets

Ph.D. student: Lifei Cheng (started August 1998)

Background: Collaborating with Profs. Biegler and Grossmann on a DOE funded project, we are looking at developing a design methodology and supporting tools to study processes from a life cycle perspective.

This project started with John Clark. John's goal was to develop methods for the synthesis of future scenarios for a process. So rather than synthesizing processes, he proposes to synthesize scenarios. He anticipated where future technology might challenge a process. He explored the use of a so-called "free step" (originally proposed by Bill Johns and his student Romero in the 1977 and 1979). If one can have any step in the process for free, then by how much would the process and its economics change? If a step allows for significant improvement, then it becomes a candidate for assessing the possibility someone might figure out how to do it. Together this information will aid one to assess the possibility such a technological breakthrough could threaten the current design.

John Clark completed an MS degree on this project in the spring of 1999. In his thesis he looked at an economic objective to assess when a new process will threaten an existing one. He devised different types of free steps that could result from a breakthrough in technology. One is a magic separation step where one removes product from a reactor that is equilibrium limited, thus allowing the reactor to completely convert the reactants. Having such a technology can dramatically alter the process design and its economics. To determine if a proposed technology breakthrough can be a threat, he synthesized a new process based on it. He then asked if this new process is viable when the current process only has to recover its operating expenses; essentially the existing process will write off its investment costs when threatened. For a breakthrough that can be a threat, one must then assess the probability the technology leads to a new process in five, ten, fifteen or twenty years. He proposed to calculate the expected value of the present worth over all the possible scenarios. The ratio of this expected value to the value if there is no risk gives one possible vulnerability index for a proposed design.

Lifei Cheng started on this project in January 1999. His work has led him to suggest designing a simulation environment in which both the process being proposed and the external environment may be modeled. The model will include stochastic variables. He is looking specifically at the modeling of the process over its entire lifetime of, say, 20 or more years. The external environment model can contain possible technology breakthroughs that may happen. One can write a process model that can respond to a breakthrough should one occur. He found several modeling systems that handle events and stochastic variables and implemented some simple models in one of them to learn about how one can model in that system.

He then demonstrated that he can model events (using ideas that Vicente Rico-Ramirez developed early in his Ph.D. project) non-procedurally. He also demonstrated that he can model queues (e.g., an order can be added to a queue to be processed later), time delays, and so forth, in a non-procedural modeling system (yes, ASCEND). The conjecture is that this approach to developing these models will be very easy for a typical modeler, a conjecture we have yet to prove. It may be hard for a person steeped in the traditions of procedural modeling at first, however, as it will represent a very different way to think. The idea is that one simply says what has to be true and not the order in which things will happen. The truth can include events happening when something starts to boil, for example, and for the system to alter its modeling equations for times that follow when that happens. You are probably thinking about this procedurally while it is being described here. The trick is to think clearly and easily about it non-procedurally. When (not if) that

becomes possible, then we can model both physical artifact and its operation in the same language. The solvers will not care which is which.

Lifei has reviewed many publications on design under uncertainty (engineering), on dynamic investment under uncertainty (economics) and on sequential decisions under uncertainty (operations research) that relate to the topic he is studying.

Solving stochastic problems: Lifei has investigated the various ways one may solve dynamic stochastic models. As noted above, these problems are recursive and have the form:

$I(t_k)$ = Minimize (over the decisions possible for the next time period)
the costs related to those decisions
\+ expected value of $I(t_{k+1})$

The demand for future time periods for product, for example, will be stochastic. Also we may describe some of the model parameters in terms of a probability distribution – e.g., the possibility that a new technology will become available. Decisions are both continuous (a flowrate) and discrete (the purchasing of new technology that may or may not occur at some time in the future). Among problems that fall in this class are inventory control problems and moving horizon control problems.

Lifei developed a small problem involving only discrete decisions and states on which he tested the various approaches possible for solving. He used dynamic programming to solve from an end time backwards to the current time. He also showed how to expand the problem to all of its equations and solve as a large simultaneous problem. He argued that often one can partition a problem into a nonstationary first few years and then a stationary problem from then on. One can solve the stationary problem first and use its solution as a boundary condition for the non-stationary part. A stationary problem is often much easier to solve.

Progress on problem formulation alternatives: Lifei examined reformulating the stochastic problem he wishes to solve. These problems always have multiple objectives. For example, posing a problem to maximize expected net present worth can lead to decisions that could, under certain future values for the stochastic variables, lead one to close the company, a result the company would not in fact want. A second objective is that the company should still be prospering 10 years. Thus a secondary goal might be to minimize the probability that some of the scenarios would have the company deciding to close down. For example, if the analysis projected a negative expected future worth along any path and if the company in fact ends up on that path, it might elect to shut down.

Solving multiple objective stochastic problems: Lifei has developed an interesting approach to solve the multi-objective stochastic optimization problem of the type described above using a dynamic programming approach. The standard approach for finding Pareto optimal sets of solutions is to convert a problem of the form

$$\begin{aligned} & \textit{Min } F1(z) \\ & \textit{Min } F2(z) \\ & \textit{Min } F3(z) \\ \textit{s.t.} \quad & g(z) \leq 0 \end{aligned}$$

into the problem

$$\begin{aligned} & \textit{Min } F1(z) \\ \textit{s.t.} \quad & F2(z) \leq a \\ & F3(z) \leq b \\ & g(z) \leq 0 \end{aligned}$$

and searching parametrically over *a* and *b* for the Pareto set. Applying this to the dynamic programming approach for solving, the objectives F2 and F3 become constraints applied at the final time. The search is to find solutions that satisfy these constraints, solving repeatedly for differing values of *a* and *b*. However, it is a bit more complicated as these objectives involve expected values. Lifei has extended the state space with two new variables per objective; the first is related to the objective and is evaluated forward in time while the second is related to the amount one will allow for the objective in the remainder of the problem – e.g., "present worth to go" or "risk to go." He shows the "objective to go" is a general reformulation trick. The search is modified as one has to allow nodes in the dynamic programming search network that may yield undesired expected values but which, when added in with other possible points, may allow for acceptable expected values for earlier points as one searches backward in time. Interestingly, the entire search over all the values of *a* and *b* can be accomplished in one backward sweep. Thus the added states enlarge the problem significantly, but the parametric search does not.

Recent progress: Lifei has formulated and solved an example problem of this type. We now have a manuscript completed and submitted that describes this work (included with this newsletter). Of real interest is the impact that risk can have on the decisions one would make. Ignoring risk, one would choose the design that maximizes expected present worth. When analyzing the decision policy this solution suggests, one finds that present worth scatters very widely and is often negative for the solution that maximizes the expected value of the present worth. If one chooses solutions to reduce the expected value of the risk and thus the expected value of the present worth, the present worth is never negative.

Art is retiring in 2003

As noted in the last newsletter, Art will be retiring officially (but not actually) in the summer of 2003, the year in which he turns 65. He will continue to improve the ASCEND system after he retires.

Visiting Researchers

Art has invited two researchers to visit for six months and for two years respectively. The one from Hangzhou, China -- Zhijiang (Jon) Shao – is one month from finishing his visit. He has developed a tool box within MATLAB to allow one to set up and solve an equation-based model in the style in which one would create and solve a model using ASCEND. The intention is to introduce that style of modeling to a wider community and to have that community then add to this tool box.

Other activities

Product Design Course: Among his current activities, Art has organized and is directing a general engineering product design course here at CMU. Taught for every term since the spring of 1999, this course encourages the participation of juniors, seniors and graduate students from all colleges. Each student works as part of a generally very diverse team on an engineering product design project. All aspects of the design of a new product or process are of concern: customer need, product function, product form, technical design, appearance, human interface design, and impact on society. Most of these projects last two terms and are directly suggested and supported by local industry or government agency. As students often take the course for only a single term, the issue of turning over a partially completed project to new personnel is a significant issue we meet head on; we grade the teams on their use of our LIRE' document management system to capture, organize and share all information for their projects.

Erik Ydstie's Group

Robust Adaptive Control Using Multiple Models

Students: Jennifer Hill (Ph.D. student started Fall '97)

Jennifer Hill developed the convergence and stability results for a new algorithm for adaptive control. The method incorporates a method that stops estimation when there is insufficient data available to perform identification. In this way her estimators only use the most reliable information, and they can be guaranteed to converge. At the same time as one estimator converges another one will be started so that several models will be generated. A logic switch will choose which model to use for control system design. The method is currently being tested in simulation studies.

The extended adaptive extended horizon controller for stabilizing the crown temperature of the SIEMEN's glass furnace has now been in continuous operation for a about two and half years. The adaptive algorithm performs much better than a well tuned PID controller since the process is nonlinear and time varying because of inherent complex dynamics, changes in operating conditions, and external disturbances. The adaptive controller retunes its performance so that optimal performance is achieved at each operating point.

Jennifer has finished the development an on-line self optimizing controller for an ELKEM Metals Silicon smelter. She uses the same estimation techniques she has developed in adaptive control research. These are combined with a Hammerstein model and a Newton based optimizer. At each step a nonlinear model of the process is estimated and the optimal operating point is approached using hill-climbing. We are currently waiting for data from the Silicon smelter to prepare on-line trials in the spring.

Distributed Simulation and Control of Process Networks

Students: Vianey Garcia-Osorio

Vianey Garcia-Osorio has tested a new approach for static and dynamic simulation of process methods in a few case studies. The method is based upon the thermodynamic stability and process network theory. The simulation 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 and has been used to simulate single process networks. 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. We have worked with an undergraduate CS minor student to streamline and optimize the code needed to interface a large number of computers over the Carnegie Mellon network

Modeling and Control Complex Chemical Reactors

Students: Dimitrios Gerorgios
Vianey Garcia-Osorio
Martin Ruzskowski

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 2000ºC and includes a fluid/gas/solid CFD model for the electrical fields, fluid flow, and chemical reaction.

Vianey Garcia-Osorio 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. She also looks at stability and overall process integration.

Martin Ruzskowski models the primary silicon production unit. This is an electric air reactor with a vapor recovery section somewhat similar to the one developed by Vianey. The primary reactions now take place between silicon, silicon dioxide, and silicon carbide rather that aluminum, alumina, and aluminum carbide. Martin interfaces this model with the solution system DASPK for solving differential algebraic equations. He will embed his model and the DASPK solution continues in an optimization shell for real time process optimization and control.

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. We plan to generalize the concept to a broader class of problems, including biological systems and crystallization processes.

CAPD REPORT SERIES

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Submitted Papers: (will be available on the CAPD website)

B-01-09
Waechter, Andreas and Lorenz T. Biegler, "Global and Local Convergence of Line Search Filter Methods for Nonlinear Programming", CAPD Technical Report B-01-09 (August 2001, revised November 2001), submitted

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B-01-11
Arora, N., L. T. Biegler and G. Heyen, "Data Reconciliation Frameworks," in *Computer Aided Process Engineering*, R. Gani and B. Braunschweig (eds.), Elsevier, to appear

B-01-12
Bartlett, R. A., L. T. Biegler, J. Backstrom and V. Gopal, "Quadratic Programming Algorithms for Large-Scale Model Predictive Control," Journal of Process Control, accepted for publication (2001)

G-01-16
Harjunkoski, I. and I.E. GROSSMANN, "Decomposition Techniques for Multistage Scheduling Problems using Mixed-integer and Constraint Programming Methods," submitted for publication (2001).

G-01-17
Jackson, J.R. and I.E. GROSSMANN, "High Level Optimization Model for the Retrofit Planning of Process Networks," submitted for publication (2001).

G-01-18
Perea, E., I.E. GROSSMANN, E. YDSTIE and T. Tahmassebi, "Control and Optimization of Supply Chains in a Dynamic Environment," *CEPAC Workshop*, Guaruja, Brazil (2001).

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