TABLE OF CONTENTS

GENERAL NEWS

Erik presented the global outlook for the solar cell industry in a conference in Tokyo in March. The focus of his presentation is the feedstock problem for Si-based photo-voltaic technology. He visited NEDO and had discussions with SHARP and Kawasaki about the feedstock problem for solar cell industry. A shortage of solar grade Silicon is predicted in the near future due to a rapid world wide expansion of the solar cell industry. In the beginning of May, Erik spent a day at AstroPower, a solar cell production company in Delaware. AstroPower and ELKEM have formed a joint venture to produce SolarGrade Silicon. In May Erik went to Norway to review the Solar Research program, from Sand to Solar Cells at NTNU in Trondheim. Erik has a position as Professor II in the Department of Materials Technology at NTNU.

Tobias Jockenhoevel and Yuen Yi Li from the Technical University of Berlin are visiting Larry's group to incorporate the barrier method into a MATLAB-based dynamic optimization package named OCOMA. This package is meant for on-line identification and control of power plants.

Masaru Noda from Kyoto University (Japan) and Daeho Ko from Yonsei University (Korea) have joined Larry's group as postdocs. Masaru Noda is investigating large-scale dynamic optimization in process engineering, while Daeho Ko is focusing on optimization of PSA systems for CO_2 sequestration.

Sarette Van den Heever successfully completed her Ph.D. degree in April, and has joined SCT Corp., a supply chain consulting firm. A number of our students are doing internships this summer. Jayanth Balasubramanian is at ExxonMobil, Sangbum Lee is at Eastman Chemical, and Edgar Perea is at McKinsey

Marta is doing a Ph.D. at the Technical University in Telemark. She has been visiting with us since January. She is returning to Norway in July. She is has been working on inventory control of particulate processes and population balance modeling of particulate systems for ELKEM ASA and the Norwegian research council. Marta was awarded the prize as the best chemical engineering student in Spain. Congratulations!

Edgar Perea is spending the summer with McKinsey consulting in Mexico to hone his skills on supply chain management problems. Vianey is working at ALCOA during the months of June, July and August on carbothermic processing for aluminum production. She attended the course offered on the FACT database system in Montreal. Martin presented a paper at the INFACON conference in Quebec on modeling the Silicon smelter as a DAE system, Dimitrios presented papers on thermodynamics and modeling of the carbothermic aluminum process in Greece. Erik presented a paper on Distillation control at the ESCAPE meeting in Denmark.

New Ph.D. students that have joined our research groups late last year are as follows: Maame Poku (Hampton University) and Cong Xu (Tsinghua University) joined Larry's group; Vikas Goel (IIT-Madras) joined Ignacio's group; John Siirola (Purdue) joined Steinar's group; Ashish Agarwal (Berkeley) joined Erik's group.

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 was held on March 26-27, 2001. The first day of the meeting consisted of overviews given by Larry, Art, Ignacio Steinar, and Gary, followed by a discussion with industrial participants, and a poster session by the students. A very successful group dinner was held that evening at the Monterey Bay Fish Grotto. The second day was devoted to final year student presentations. We are especially grateful for the very positive feedback on this meeting. Next year's meeting is scheduled for March 25-26, 2002. If you have any additional thoughts or suggestions, please let us know.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* took place on June 21-27, 2001. This year we were very pleased with the outcome of our course. We had 11 attendees from around the world, both from industry and academia. The course has been extensively revised and includes the following modules:

a) Conceptual Design - taught on Thursday and Friday (June 21-22), 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 23 and 25), 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 26-27), with focus on differential/algebraic models for real time optimization and parameter estimation, and on mixed-integer programming models for process scheduling and supply chain management.

The course included extensive workshops where participants obtained hands-on experience with various software packages. Course materials included extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." Dates for next year's course have not been set yet. Nevertheless, 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 the next issue of the CAPD newsletter, including the reprints and papers, will be distributed in electronic form. All members will have access to these 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 are initiating 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. Both are described below.

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 from the Technical University of Berlin on the OCOMA package, which incorporates these dynamic optimization strategies using MATLAB interfaces.

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 project with Dow dealing with optimal multiperiod operation of a network of polymer plants. **Jose Caballero**, whose paper on the synthesis of thermally integrated columns has been published, is continuing work in this area.

In the area of optimization **Sangbum Lee**, has developed a global optimization method for generalized disjunctive programming models to rigorously handle nonconvexities that are due to nonlinear equations. Major applications have been in the area of blending. Sangbum also made a very interesting discovery regarding tightness of improper disjunctions when represented through the convex hull equations. **Aldo Vecchietti**, has completed the version of LOGMIP for handling disjunctions in linear problems.

In the area of planning and scheduling **Jayanth Balasubramanian,** has developed a new approach for scheduling under uncertainty that relies on concepts of interval arithmetic and fuzzy sets and numbers. Compared to traditional probabilistic approaches the proposed method yields similar results with order magnitude reductions for the optimization. **Sarette Van Den Heever**, completed the first part of a project with Air Products, dealing with the multiperiod optimization of hydrogen pipelines for which she

developed planning and scheduling models. **Iiro Harjunkoski** is continuing that work. He has also developed a novel set of cuts for a hybrid scheme (MILP and Constrained Programming) for multistage batch scheduling that leads to order of magnitude reductions in computations. **Christos Maravelias** has been investigating new formulations and efficient solution methods for the resource constrained scheduling problem for new product development. A manuscript describing his work on integrated testing and manufacturing is enclosed. **Martin Houze** has a project under way in collaboration with Totalfinaelf in the area of optimal catalyst management for which he has developed a multiperiod MINLP model. In the area of supply chain optimization, **Edgar Perea,** under the supervision of Ignacio and Erik, has developed 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 traditional control objectives (e.g. minimizing deviations). Finally, **Gabriela Garcia** has started to develop a framework for transferring the PC interfaces as web-based interfaces.

In **Steinar Hauan's** group, **Warren Hoffmaster**, in his pursuit of feasibility analysis in reactive separation processes, continues to work on a design decomposition strategy. It seems that all possible pieces of reaction-separation equipment may be represented by carefully chosen combinations of only three elementary pieces: Non-reactive, extractive, and reactive. The key point is to work with reachable regions in parts initially left unconnected to each other to reduce complexity but keep generality. Warren has developed the tools necessary to systematically subdivide the initial conditions for which different approaches must be used to address reachability. The non-reactive case has been solved while advances have been made on the reactive and extractive building blocks necessary.

John Siirola has just started his work on agent-based systems for distributed, asynchronous process design, but has implemented two systems. The first is a proof of concept and deals with models for market information leads to significant impact on the economics for both consumers and producers. The second is more substantial and deals with optimization of multiple, mathematically 'nasty', objective functions in a non-convex domain. The initial runs are being completed as this is written and the first set of full-scale results is expected in July. For this purpose, we expanded our Beowulf computer cluster by adding 20 more cpu's in the end of May.

Jan Morbach and **Reiner Jorewitz** have been working on simulation of 3-dimensional reactor with laminar flow and forced mixing. Their results show that PDE solution of the reactive flow problem quickly becomes computationally prohibitive, but also suggest several possible reactor designs. The effort in microscale gravimetric detection of biomolecules continues with collaborators in BME, ECE and Biology and a laser rapid prototype system has been installed in the lab.

Murni Ahmad has been working with **Todd Przybycien** on flexible design of biochemical processes. After giving birth to her second child, she continues work on a modular optimization formulation of a 2-phase aqueous system for protein separation.

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. Lifei has a summer position with Exxon/Mobil and will return to CMU in mid August.

John Siirola, working with **Steinar Hauan** and **Art Westerberg**, is demonstrating the synergy of using many types of agents to solve complex optimization problems.

A visiting faculty member, **Zhijiang (Jon) Shao** from Hangzhou, China, has just arrived. He will be working with **Art Westerberg** on modeling issues. He expects to be here until the first of this next year.

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 started Fall, 1996)

Roscoe Bartlett 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. 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 was presented at the First CSRI Workshop on PDE-based Optimization and is listed below.

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. Moreover, it 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.

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 the rSQP FORTRAN code to adapt it to larger NLP problems. 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 spending the summers at Sandia to implement and test these ideas.

During the past summer, 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 was presented at the First CSRI Workshop on PDE-based Optimization and is listed below. Finally, Cong Xu recently joined this project and will also be investigating optimization problems arising in fluid dynamics and transport phenomena using Smooth Particle Hydrodynamics (SPH).

Barrier (Interior Point) Methods for Nonlinear Programming

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

This project extends the previous project by developing an efficient strategy for solving nonlinear programs, generated by rSQP, with interior point (IP) methods. This approach works either in the full space or can take advantage of the particular rSQP decomposition (choices of Z and Y). However, 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 spent the last summer working with Prof. J. Nocedal at Northwestern on the direct solution of the NLP with barrier methods. Here we are 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. In particular, 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 is currently in preparation and will be listed in the next newsletter. 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 800,000 variable problems were solved in about 66 CPU minutes on an 800 MHz computer. Problems of over twice this size have also been solved recently. Moreover, this approach has been linked to a number of packages including DynoPC, OCOMA and AMPL. Finally, the interface of this approach to large-scale modeling packages and further testing is described in a paper listed below that was presented at the First CSRI Workshop on PDE-based Optimization.

Mathematical Programs with Equilibrium Constraints (MPECS)

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

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 of the form 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 will be 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. Also, 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.

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, Maame Poku has recently joined this project and is 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: **Daniel Osorio (Pontifical Universidad Catolica de Chile)**

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. Daniel Osorio, a visitor from Chile will be working with Yi-dong on optimization applications for batch distillation in the beverage industry.

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 a 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. At present, no satisfactory optimization strategies have been developed that can deal with these models. Ling Jiang is continuing her work on this project. She is spending the summer 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. These models have strong hyperbolic and parabolic components and require special mass conserving discretization strategies to convert them to DAEs. Termed flux limiters, these discretization allow the accurate tracking of steep fronts and discontinuities that frequently arise in PSA systems. Ling has successfully simulated cyclic steady state conditions in a small PSA unit, using Newton-type solvers. From this point she has demonstrated a framework that includes constrained simulation problems and design optimization problems on a number of PSA examples. Her work this summer is to refine these methods so that more efficient methods are developed.

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.

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. A paper that describes this approach is listed below.

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 is investigating 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.

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

Status: *On hold*
Student: **Jennifer Jackson [Ph.D. , started Jan 99]**
Collaborator: **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. This project is temporarily on hold, until Mariana Bartfeld arrives from Argentina. 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:

Jennifer Jackson: Reactive Distillation
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 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. She extended her model to consider potential heat exchanges in each try. 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. The second problem that Jennifer has solved is the production of ethylene glycol from ethylene oxide and water, with side reaction of ethylene oxide and ethylene glycol to form diethylene glycol. With a maximum of 40 potential trays the problem involved 38 discrete variables, 1705 continuous variables and 1593 constraints. The disjunctive problem was solved in 5 major iterations requiring a total of 55 minutes of computation. The predicted design involves 31 trays with 19 feed trays. The reactive trays were located between trays 5 and 31.

Juan Reyes: Liquid-Liquid extraction
Juan Reyes developed a 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. In one of the examples Juan considered the separation of a stream consisting of water, acetone and acetic acid, in which the objective was to separate acetone using pure chloroform as the solvent. Using special correlations that Juan has developed in Spain for equilibrium, for a 90% recovery of acetone, Juan was able to synthesize a countercurrent configuration of 6 stages, in which there are two lateral extractions. The problem involved 10 boolean variables, 350 continuous variables and 547 constraints, and was solved in about 570 secs (Pentium II). Juan is currently exploring the use of global optimization techniques for this problem. A copy of his ESCAPE paper is enclosed.

Jose Caballero: Thermally linked columns.
Jose addressed the synthesis of thermally coupled distillation column configurations to separate non azeotropic multicomponent mixtures containing N components. He showed that for sharp separations of an N component mixture it is possible to develop a superstructure that takes into account all the possibilities, from thermally linked systems with only one reboiler and one condenser, to sequences with only conventional columns (2(N-1) condensers and reboilers). All the partially thermal linked superstructures are included. The superstructure is systematically generated using the State Task Network (STN) formalism. Jose modeled the superstructure using Generalized Disjunctive Programming using shortcut models. Jose used a modified version of Logic Based Outer Approximation algorithm to solve several example problems that were applied to hydrocarbon mixtures. The interesting part of Jose's results is that the column configurations he synthesized even for these ideal systems involved side-rectifiers or side-strippers, or led to Petlyuk column configurations. Jose is currently exploring the inclusion of heat integration in these columns. A copy of his ESCAPE paper is enclosed.

Operational Planning and Retrofit Design in Process Networks

Students: **Jennifer Jackson [Ph.D., started Jan 99]**

New Development: *Multiperiod model in joint project with Dow*

Jennifer's project has been concerned with developing highlevel optimization models for process modifications. Her work has recently been redirected to a project with Dow, dealing with multiperiod optimization of a network of polymer plants.

The initial problem that Jennifer considered can be stated as follows. Given is an existing network of processes 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. In each year there is a limit of capital investment for retrofit projects. The problem consists in identifying retrofit projects for those processes that will yield a maximum improvement in the Net Present Value. One of the challenges in this problem is how to estimate the effect of the various types of process modifications, without having to carry out a very detailed study in each plant. Jennifer developed a generic linear model for processes in which the various types of modifications can be incorporated. Tools such as attainable regions and pinch analysis are being explored to help estimate the benefits and limits of improvements. 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 has also been looking at two related issues. One is 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. The second issue that Jennifer is investigating an alternative

representation of the disjunctions, which leads to bilinearities that can be replaced by exact linearization techniques.

Since February, Jennifer embarked on a 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 has demonstrated on this project the advantages of GAMS over Excel, which was initially used to address monthly productions. Jennifer is currently exploring the extension of this model to a supply chain optimization problem involving multiple sites and with the possibility of performing capacity expansions.

Algorithms for Nonlinear Disjunctive Programming

Students:	**Sangbum Lee [Ph.D., started Jan 98]**
Research fellow:	**Aldo Vecchietti [Ph.D., completed Aug 2000]**
New Development:	*Handling of nonlinear equations; applications to blending* *Discovery of tightness properties of convex hull for improper disjunctions*

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 tighter lower bounds than the ones that are obtained when the above GDP is converted into an MINLP with "big-M" constraints. This NLP relaxation can be used in three different ways:
I) To reformulate the above GDP as an MINLP, which can then be solved with methods such as outer-approximation, generalized Benders and extended cutting plane.
II) To develop a logic based outer-approximation algorithm in which the NLP subproblems only involve the active terms of the disjunctions, and where the MILP master problem is constructed by linearizing the NLP relaxation, as opposed to linearizing the functions themselves and then applying the convex hull.
III) 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, including problems related to process networks, optimal positioning of new products, and batch design. The main conclusion in all these applications is that significantly improved lower bounds were obtained in most problems compared to the traditional MINLP models, which often translated in more efficient solutions.

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 problem involving 6 batch tasks, 7 equipment and 6 products the GDP involves 53 boolean variables, 105 continuous variables and 13 disjunctions. The algorithm found the rigorous global optimum ($726,205) in about 2 minutes. In contrast, applying DICOPT to the MINLP formulation to that problem yields a suboptimal solution of $787,983.

Based on the work on global optimization, Sangbum has addressed the case when nonlinear equations are involved in the disjunctions. In this case nonconvexities are often present, and may cause great difficulties as is for instance the case of bilinear equations for pooling and blending applications. The idea in Sangbum's approach is to replace each equation by two inequalities. The analysis of each of them may indicated the presence of nonconvexities in which case convex envelopes or valid underestimators are used. An interesting result that came out, is that it is possible to show that it is better to apply these understimators in each term of the disjunction, rather than use new variables to replace nonlinear equations with linear equations in the disjunctions, and then apply the underestimators outside the disjunctions. The reason is that the former can be shown to yield tighter relaxations. Once the replacement is performed, the procedure reduces to the global optimization work that Sangbum had developed for the case of inequalities. Sangbum applied this method to a number of problems dealing with blending, and that involve discrete variables, for example to set up minimum amounts to be blended, and to decide which tanks to use or not. Since these problems involve bilinearities, the McCormick underestimators were used. Sangbum is in the process of writing this manuscript, and solving additional test problems.

In yet another part of this project, Sangbum looked at a question that had been addressed by Aldo Vecchietti, namely characterization of disjunctions, and the impact of relaxations for the big-M and convex hull relaxations. One way to characterize disjunctions is to divide them 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. 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. In plain words, the algebraic expression of the convex requires 0-1 variables, and it is these that make the difference. Sangbum has a small geometrical example that illustrates this property very clear. Sangbum is in the process of writing this paper, where he has also included a section on a cutting plane algorithm as an alternative to using the explicit equations of the convex hull.

Finally, if it were not enough, Sangbum had a small diversion in his research. In collaboration with Michael Domach, a faculty from Chemical Engineering in bioengineering, he was involved in the problem of finding all the alternate solutions of an LP related to a metabolic network. While there are a several special purpose methods reported in the literature for finding all alternate optima in an LP, there are no codes that

are readily available for this problem. This motivated the development of 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 has been applied to the LP of a metabolic network involving about 50 variables and constraints. Typically these problems involve between 10 and 30 alternate optima that our proposed method can rigorously find. This work has now been implemented by a student from Mike Domach, and is used as a screening tool for conducting NMR experiments. The copy of the manuscript that just appeared in *Metabolic Engineering* is enclosed.

Aldo Vecchietti: LOGMIP and modeling issues

The project by Sangbum is being complemented by Dr. Aldo Vecchietti from INGAR in Argentina. The man thrust of the work by Aldo has been the developments of LOGMIP, as well as the analysis of alternative models for disjunctive programming. An interesting contribution in Aldo's work has been the analysis of relaxations of disjunctions and big-M constraints, as well as a characterization of disjunctions for which one can determine a priori whether or not the convex hull relaxation will lead to tighter formulations. This work is currently being integrated with the paper with Sangbum. Aldo has also produced 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. In each of these blocks of constraints can be specified. Aldo has recently shown that the IF THEN ELSE construct can be applied to embedded disjunctions. 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. Therefore LOGMIP will be able to handle implications by converting them internally into disjunctions. In fact one example from ILOG was totally transformed into a GDP and successfully solved with LOGMIP in one single iteration.

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. Our idea is to first provide this capability of reformulation for MILP problems. The motivation is that a user be able to express constraints in semi-symbolic form, and have LOGMIP do automatically the reformulation into an MILP.

MINLP and Disjunctive Multiperiod Optimization Methods

Students: **Susara van den Heever (Ph.D. started January 1997-completed April 2001)**

New Developments: *Completed Ph.D. thesis*

We briefly summarize Sarette's Ph.D. thesis (expect the last chapter). Sarette's project dealt with the solution of mixed-integer *nonlinear* multiperiod models. The major focus of application in her work was the design and optimization of oilfield planning problems, which was conducted in collaboration with Mobil Technology, and then ExxonMobil.

Sarette first considered a general model and solution method for multiperiod optimization problems. She developed a general disjunctive formulation that considers as major discrete decisions selection of design (synthesis), operation of unit, and capacity expansion. This model involves embedded disjunctions that reflect the decisions of design, operation, and capacity expansion. It also has as particular cases the "traditional" multiperiod design problem (i.e. no operation, capacity expansion), the capacity expansion planning problem (no 0-1 variables for operation), and the operational planning problem for a fixed design. Sarette developed a bilevel decomposition method that consists of an upper level that is concerned only

with the design variables and a lower level that is concerned with the operation and capacity expansion. The upper level problem requires the definition of a special problem that exhibits bounding properties, while the lower level problem is simply the original disjunctive program for a fixed design. Each level is solved with the logic-based MINLP method. This method proved to be very successful as it allowed the solution of process networks problems with up to 25 periods, and retrofit design of multiproduct batch plants with 10 time periods.

Sarette also developed a nonlinear model for the offshore oil facilities planning problem in collaboration with Sriram Vasantharajan and Krisanne Edwards from ExxonMobil. The nonlinearities arise for the predicting the pressure in the reservoirs and the corresponding cumulative production flow of gas and oil. Using ideas of global optimization, Sarette used underestimators to increase the likelihood of finding the global optimum with an MINLP formulation. Since the computing times were rather high, she investigated a strategy that makes use of the bilevel decomposition and relies on aggregating time periods in the upper level problem. Using this method Sarette was able to solve problem with up to 25 wells and 24 time periods. Her method requires about 20 minutes of computation compared to about 6 hours that are needed when DICOPT is used to directly solve the problem.

Sarette also addressed a different version of the problem 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. The handling of these economic terms is quite complex because they are given by complex rules that involve tax incentives for long term investment. These rules are normally given in terms of gross revenues and investments, which incur different percentages of royalties depending on the net earnings. Most optimization models in the past have ignored these royalties due to their complexity since their relaxations are very poor and the size of the problems is greatly increased. To solve large problems Sarette investigated a new a specialized algorithm based on Lagrangean decomposition. The basic idea behind this decomposition is to exploit the structure of a model in which few variable link separate sets of constraints. By duplicating these variables, each constraint set contains a different variable, thus decomposing the model. In the case of oilfield infrastructure planning, by duplicating the pipeline variables, and assigning one variable to each well platform, the model becomes completely decomposable over each platform. The constraints that link the platforms, i.e. the ones that sets the duplicate variables equal, are removed to facilitate decomposition of the model, and replaced with a penalty in the objective function. This penalty is the product of the deviation in the removed constraints, and the associated Lagrangean multipliers (hence the name "Lagrangean decomposition"). The largest problem Sarette solved consists of 16 well platforms, with a choice of 23 pipeline connections, to be solved over 15 years and the optimization model consists of 12696 constraints, 7633 continuous variables and 919 discrete variables. When attempting to solve only half this model in the full space, no solution could be found in more than 3 days, while with Sarette's proposed Lagrangian decomposition algorithm the optimal solution was found in about 33 hours, yielding a 5.7% increase in the NPV compared to the case without complex economic rules ($64 million improvement). This work is due to be published by *I&EC Research* within the next few months.

Optimal Design and Planning of Oilfield Infrastructures under Uncertainty

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

New Developments: *Initial efforts to reduce dimensionality*

Vikas is a first year student who will be continuing the efforts of Sarette in the area of oilfield planning. The major focus of Vikas will be the handling of uncertainties. The two biggest sources of uncertainty in this problem 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. 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 demonstrated that using a Lagrangian decomposition scheme one can aggregate the multipliers 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. Vikas has tested this strategy on a very small process network problem, obtaining very good results. The effectiveness in the oilfield problem, and the establishment of bounding properties of this method remains to be seen.

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]**

New Development *Decomposition strategy for integrating planning and scheduling*

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 is currently continuing this project. He is first revisiting different options for handling the difficult nonlinearities that give rise to non-differentiabilities. He is also concentrating on the scheduling part to see if one can beyond the solution of a single period problem.

Scheduling of Batch and Continuous Multiproduct Plants

Postdoctoral fellow: **Iiro Harjunkoski (started September 1999]**

New Development *Cuts for MILP/CLP model for multistage batch plants*

Iiro has undertaken several projects. One of them has been to continue the work initiated by Vipul Jain for integrating CLP (Constrained Logic 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 CLP 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 CLP problem for the latter in the spirit of Vipul's hybrid strategy. The key difference is that generating tight cuts for the MILP in this problem has turned out to be surprisingly. One can of course use the standard integer cut, but the problem is that it is very weak. As reported in the last newsletter Iiro found a 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 computational on several examples were very encouraging. For instance on a problem with 8 orders, 3 stages and 6 equipment the MILP with CPLEX required 6056 secs, while the proposed hybrid strategy, using CPLEX and OPL, required less than 4 seconds to be solved to optimality. While the results have proved to be encouraging, Iiro discovered a counter-example to the cuts he had derived. Although the discrepancy is rather small, it would of course be desirable to obtain the rigorous cuts that are valid in all cases. This is the question that Iiro is currently addressing.

Regarding the collaboration with Kvaerner, Iiro has largely terminated the work of scheduling of a steel plant. This problem contains a large number of chemistry-, geometrical- and scheduling rules. 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]

Status: Development of new approach based on interval arithmetic, fuzzy sets

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 extended this branch and bound procedure to flowshops with UIS policy. He has also to extended it 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. For an example with 8 products and 2 stages the exact value of the expected completion time for rectangular distributions for each processing time was 265.24 hrs. With the proposed discretization scheme the approximate value was 265.23 hrs.

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. However, it was clear that extensions to multistage systems would be very hard, and generalizations that might allow tackling the scheduling for new product development would be even more difficult.

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 equivalent to interval arithmetic where the major result that one can obtain are lower and upper bounds for the completion time for a fixed schedule. Using triangular fuzzy numbers, the equivalent to the expected completion time reduces to the average completion time integrated over all parametric intervals that are centered to the center point, and with deviations proportional to the bounds of the completion time. To extend this approach to optimization 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 new product development, with 9 and 65 tests, and in which the objective was profit maximization. The 9-test problem can be solved in 600 secs or 7611 secs, depending on the number of points for the approximation that are used for the integral (7 and 21, respectively). The 65 test problem was solved in 324 secs or 2786 secs, using 7 and 21 points, respectively. It should be noted that although these times may appear to be somewhat high, optimizing a schedule of new product development with uncertain task durations is an extremely difficult problem. Jaynath is currently completing the study of numerical tests, and is applying the method to flowshop and multistage batch plants.

Integration of Product Testing and Planning of Batch Manufacturing Facilities

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

New Developments: *Exploring improved solution method 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 are also 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. The reason this problem is significant in practice is that currently no systematic methods for deciding when to start preliminary design of the batch plants, nor of knowing whether it is best to use existing facilities to accommodate new products or building a new plant. A major limitation at the moment is that the model considers the process development part in a simplified way by treating it as a task of fixed duration that has to precede the design of the plant.

Based on the previous 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 has been 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 experience on a biotechnology application has been encouraging. In that problem it is assumed that a plant involving 4 stages 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 4 hours to solve this problem; with Lagrangean relaxation only 10 minutes. The solution to this problem indicated a schedule for testing over a 22 month period, as well as a plan for capacity expansion of the plant over a 3 year period starting after 10 months, which is when the first product can be launched under the optimistic scenario. The solution also indicates the optimal plan that is to be implemented in each scenario. We are currently discussing this project with Bayer and Bristol-Myers Squibb in order to get their feedback. We enclose the manuscpript that Christos has completed recently on this work.

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, Benders decomposition and branch and cut on a 65 test problem. Whilke results on these methods are still inconclusive, an encouraging trend is that compared to the CPU times that Vipul required to solve his problems, by simply using the same solvers and faster PCs 3 years later, the times of his problems have been reduced by one order of magnitude. Nevertheless, exponential growth is still experienced when the number of testrs becomes too large.

Supply Chain Dynamics and Control

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 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 flow 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. Therefore there is interest in determining the accumulation of inventories at each point of the supply chain. 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 corresponds mathematically to the solution of 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 was then able to analyze 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). Edgar has recently studied the effect of selecting various gains, as well as specifying various types of delivery rates. For the gains he concluded 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.

Edgar has been investigating the incorporation of optimization in the dynamic model for the supply chain, both 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 model is optimized together with the schedule and inventory levels. Since this has proved to be a very hard problem to solve, he has investigated an approach that uses a rolling horizon technique, such as the one used in Model Predictive Control, to find the control laws to maximize an objective function for the system. Since the control laws for the distribution channels and the manufacturing sites are found simultaneously, we can capture all the interactions within the system and find better solutions. The model, hybrid in nature, can be simplified to a DAE system by imposing some constraints. Moreover, either by using profits or infinite norm for customer satisfaction level as the objective function, the system is simplified to a sequential solution of MILPs. Initial results have been quite encouraging. An interesting question that Edgar is investigating is how to effectively update the successive MILP subproblems that are solved with the rolling horizon strategy.

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. An interesting question that we are still trying to resolve is whether it is possible to consider a cyclic policy given the varying demands during the year. Martin is currently performing parametric tests withy the MINLP model to better understand the trade-offs involved in this problem.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: **Gabriela Garcia (started March 2000)**
Collaborators: **Dr. Zdravko Kravanja, Univ. Maribor, Slovenia**

New Developments: *Initial Development web interfaces*

Gabriela has been starting to develop 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 wenintranet system.

Gabriela has also recently completed the interfaces WATER that 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. The method accounts for all possibilities of mixing and splitting the streams. Gabriela has also completed the interface EXTRACTOR that is based on the work of Juan Reyes Labarata for the synthesis and optimization of liquid-liquid extraction systems. This program determines the number of stages splits of feeds and feed-stage and extraction-stage location. The program is currently restricted to handling four components: acetone. Chloroform, acetic acid and water. Other recently completed interfaces include NETCHAIN, which deals with supply chain optimization for process networks with flexible processes which is based on the work of the visitor Jin-Kwang Bok from KAIST. The other interface is DECAY, which is based on the work by Vipul Jain for the cyclic scheduling of parallel furnaces that exhibit decay in the conversion due to coking. Gabriela has also completed the development of UTILPLAN, a program for multiperiod planning of utility plans, in which major decisions involved are the on/off status of equipment given that demands vary at each time period. The solution method is the shortest path algorithm coupled with synthesis of the network of events through MILP developed by Ramesh Iyer.

Zdravko Kravanja has reimplemented the old code PROSYN into the new code MIPSYN that is PC-based and that makes direct use of the recent developments in disjunctive programming. 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

Warren has concentrated on the next part of his decomposition strategy: Extreme conditions and reachable regions in cascade sections with chemical reactions. The concepts of iso-reaction and iso-reflux pinch point curves represent a generalization of theory known from non-reactive separation systems and is expected to play a vital role in the final solution. However, the results themselves are complex -- even for the simplest possible systems -- but the examples studied are chosen so they appear as subparts of any realistic case. Further, they reveal geometrically when and why currently known design algorithms fail. A classification system based on the topology of non-reactive VLE manifold combined with difference point considerations

is in the works. This is expected to allow the a priori selection of methods used to determine the reachable product regions.

Microscale process design

Students: Jan Morbach, Reiner Jorewitz (Achen exchange students)

Collaborators: Todd Pryzbycien (Biomedical Engineering), Kaigham Gabriel (Electrical & Computer Engineering), Victor Weedn (Biology)

BACKGROUND

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

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

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

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

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

Jan and Reiner have been doing a one-semester project for numerical simulation of microscale reactors in 3-D. As most attempts at solving the reactive flow problem directly fails or becomes intractable as inner loops in a design optimization strategy (more than 5gb memory or 1 week of cpu time), alternative approaches were sought. With the assumption of constant density, the chemical reactions may be superimposed on non-rective flow profiles by spline fits (Jan) or special interpolation routines (Reiner). As a result, computer time was cut by more than one order of magnitude and yielded reasonable results for a range of input conditions and geometries.

For molecular detection, Kaigham Gabriel's group has created four prototype polymer membranes with embedded electrodes on a standard silicon chip. Experiments by Angela Wilcox (a 3th year PhD student in Todd's group) are in progress to find the best way to reliably functionalize the membrane surfaces with protein receptors. We have also purchased and set up a 3-D laser engraving tool to be used to create microscale flow cells in connection with the gravimetric membranes. A 1st year PhD student is expected to join this project in the Fall of 2001.

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 had a baby (Nabil) in April, but will continue her work in the summer.

Agent-based, Asynchronous Process Design

Student: John Siirola (PhD, started Jan 2001)

BACKGROUND

Co-advised by Art Westerberg, John is studying how to deal with design problems for which deterministic algorithms are either unknown or associated with computationally prohibitive cost. The goal is to use a coordinated set of individual "solution agents" to produce the best possible design in a fixed amount of time for a given level of computing power.

Our paradigm is that a collection of principally independent – but collaborative -- algorithmic agents working in parallel may search a substantially larger and more complex design space than single-threaded approaches. In this context, both direct and stochastic collaboration is investigated.

Our strategy has three algoritmic 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 implemented the basic proof-of-concept modules for distributed task coordination and database operations. Agents are written in GAMS, Perl, C and Matlab and communicate through a standard, central SQL database. All deterministic agents are highly parametrized in the sense that their individual and combined behavior in the system may be dynamically altered through self-evaluation and meta-agents. Experiments are in progress on how to efficiently share partial solutions between algorithmic methods, how to avoid repeating similar (but not identical) calculations and how to identify and incorporate heuristics into the overall solution procedure.

The upgrade of our Beowulf computer cluster continues: We now have 27 cpu's on a custom version of RedHat Linux with a scalable infrastructure as well as easy installation and maintenance. This is less than originally planned, but the limit has been imposed by transient issues related to power and cooling. The expansion plan has been funded by the National Science Foundation and further upgrades are planned in the Fall using a mix of Intel (P4) Xeon and AMD Athlon SMP cpu's.

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.

Recent progress: 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

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

into the problem

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

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. 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.

Lifei has extended the example problem he solved earlier to demonstrate these ideas.

Agent-based large scale optimization
Ph.D. student: John Siirola (started August, 2000) (codirected by Steinar Hauan)

Background: John is looking at 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. 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. 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 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?

Current 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. It also has differing amounts of delay time built in to emulate agents that take a long time to complete their analyses. This objective function is readily set up to be evaluated over any number of independent variables. John has created several types of agents. For optimization, he has gradient-based hill climbing, simulated annealing and genetic algorithms. He also has a "look for places where there is a paucity of points" algorithm. His first testing is to solve using all agent types. He will then remove the different types one at a time to watch the degradation of the system performance in solving. Preliminary experience demonstrates very clearly the synergy we expected to see.

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. During the time that remains, he will be involved in the following activities.

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 -- just arrived.. His interest is in modeling. The other will be from Argentina and has an interest in information technology.

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.

ASCEND: When he retires, his plans are to continue to have excellent computing facilities on which he will work to extend the ASCEND modeling environment, along with major help from former graduate students. To that end, he is spending time this term "getting inside" ASCEND.

Erik Ydstie's Group

Robust Adaptive Control Using Multiple Models

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

Jennifer Hill has developed 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.

Jennifer has developed an adaptive extended horizon controller for stabilizing the crown temperature of the SIEMEN's glass furnace. The controller has been implemented on the FISHER control platform; it has been in continuous operation for a about a year. 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 also developed an adaptive predictive controller for glass temperature control. The algorithm uses feed forward from several measured disturbances; it incorporates process constraints and uses the adaptive stopping technique to avoid parameter drift and bursting. The algorithm has been tested in a simulation study of an industrial scale glass process.

Jennifer is currently developing an on-line self optimizing controller for an ELKEM Metals Silicon smelter. She uses the same estimation techniques she has developed in her previous 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.

Distributed Simulation and Control of Process Networks

Students: Vianey Garcia-Osorio

Vianey Garcia-Osorio has developed a new approach for static and dynamic simulation of process methods. The method is based upon the process network theory developed by Duncan. 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.

Modeling and Control Complex Chemical Reactors

Students: Dimitrios Gerorgios
Vianey Garcia-Osorio
Martin Ruzskowski

We have started a modeling group for complex chemical reaction systems. 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 will be 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. We plan to generalize the concept to a broader class of problems, including biological systems and crystallization processes.

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