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GENERAL NEWS

Erik Ydstie is invited by the Norwegian export council to go on a state visit to Japan in the end of March. He will travel with the King and the Queen of Norway to talk about the Solar Cell Research that is taking place in Norway. The focus of his presentation is the feedstock problem for Si-based photo-voltaic technology.

Art Westerberg is on sabbatical this term. The last newsletter indicated he would be in China for April and May. Due to personal reasons, he had to cancel this trip. Thus he is spending most of his time working at his home. His goals are two: to dig deeply into the ASCEND software so he can create new features in it and to start on a book to report the work that the *n*-dim group has done in the area of information technology.

Marta Diez is visiting from Norway until July this summer. She is working on control of particulate processes and population balance modeling of particulate systems for ELKEM ASA and the Norwegian research council.

Martin Houze from France (Lyon and Nancy) has joined Ignacio's group to work on a project with Elf Atochem in the area of optimal policies for catalyst replacement.

Students who have successfully completed their Ph.D. proposals are as follows: Nikhil Arora, Lifei Cheng, Gregory Itle, Jennifer Jackson, Dan Margolis, Dan Milam, Martin Ruszkowski.

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.

NEW MEMBERS

We would like to welcome Kraft Foods as a new member of the CAPD consortium. The representative for Kraft is Dr. Walter Ley. As with all of our members, we look forward to rewarding research interactions with Kraft.

2001 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on March 26-27, 2001. The first day of the meeting will consist of overviews given by Larry, Art, Ignacio Steinar, and Gary, followed by a discussion with industrial participants, and a poster session by the students. There will also be a dinner that evening at the Monterey Bay Fish Grotto. The second day is devoted to final year student presentations. Last year the feedback we received was extremely positive. If you have any additional thoughts or suggestions, please let us know.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* will take place on June 21-27, 2001. The course has been extensively revised and includes the following modules:

a) Conceptual Design - to be taught Thursday and Friday (June 21-22), will focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.

b) Optimization - to be taught on Saturday and Monday (June 23 and 25), will focus on modeling and algorithms for nonlinear programming and mixed integer programming including disjunctive programming and applications to process optimization.

c) Process Operations. To be taught on Tuesday and Wednesday (June 26-27), will 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 has been extensively reorganized and includes extensive workshops where participants obtain hands-on experience with various software packages. The course also includes extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in attending this course, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu

ONE-DAY TOPICAL MEETING

The CAPD is considering a one-day topical meeting in the fall of 2001. The meeting would be for CAPD industrial members and would be devoted to a single research area. Presentations and discussions would highlight research within the CAPD as well as industrial problems and approaches.

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 will be cataloging these reports on the web sites mentioned above. This will also allow 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**) and will include PSA systems (**Ling Jiang**) as well as other fluid flow systems (**Cong Xu**). Currently, **Andreas Waechter** is developing and refining barrier (interior point) NLP method, called IPOPT, based on many of these SQP concepts. This has been used to solve problems with over 500,000 variables. In parallel to this effort, **Roscoe Bartlett** is developing a C++ environment for rSQP that incorporates a number of specialized decomposition strategies and high levels of abstraction. 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 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, Bill has 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 busy writing or revising manuscripts. Some of the major developments are the following:

In the area of process synthesis **Jennifer Jackson** has completed disjunctive optimization models for reactive distillation. Her models determine the number of stages, feed tray locations, and reactive trays. She has obtained the results for the reaction of 2-pentene to form 2-butene and 3-hexene, and for the production of ethylene glycol as described in the enclosed manuscript. **Juan Reyes**, a visitor from Spain, has completed work in the area of superstructure optimization for liquid-liquid extraction systems.

In the area of optimization **Sangbum Lee**, has developed a branch and bound method for the global optimization of generalized disjunctive problems (GDP) that involve nonconvex functions (bilinear, linear fractional and concave separable). He has recently done theoretical work to prove basic properties on the relaxation of the GDP for the convex case.. **Aldo Vecchietti**, has also made some progress in the development of the new version of LOGMIP that can handle disjunctions through the use of IF ..THEN.. statements. The current emphasis is on linear problems.

In the area of planning and scheduling, **Iiro Harjunkoski** in collaboration with Kvaerner completed an implementation of a decomposition strategy for a large-scale scheduling model for steel manufacturing that is described in the enclosed manuscript. The decomposition relies on grouping orders in smaller sets, which are first solved as a flowshop problem, and then joined through a jobshop MILP. Theoretical lower bounds can be easily computed, which Iiro found to be within 1-3% of the optimum. Iiro has also developed a hybrid scheme (MILP and Constrained Programming) for multistage batch scheduling. **Jayanth Balasubramanian,** has completed the development of a new branch and bound method to

optimize the expected completion time in flowshop plants with uncertain processing times. He method, which is described in the enclosed manuscript, relies on a number of interesting lower bounding properties that lead to the examination of order of magnitude smaller search spaces compared to conventional approaches. **Sarette Van Den Heever**, who has been working in the planning and design of offshore oil field facilities in collaboration with ExxonMobil, finished the development of a novel Lagrangean decomposition method for incorporating royalties in the optimization of these systems, an objective function which greatly increases computation time. In collaboration with Air Products, she is currently involved in the multiperiod optimization of hydrogen pipelines in which she has developed planning and scheduling models. **Christos Maravelias** has essentially completed a comprehensive optimization model for the simultaneous product testing and design and planning of batch manufacturing facilities, a problem that arises in pharmaceuticals and agricultural chemicals. He is currently completing a manuscript describing this work. In the area of supply chain optimization, where Ignacio, Erik Ydstie and **Edgar Perea** have been collaborated with Unilever in the development of a dynamic model for a manufacturing-distribution-retail system. A number of detailed issues have been analyzed including rates of deliveries and selection of gains in the controllers. Way is under way to incorporate optimization through Model Predictive Control. Finally, **Gabriela Garcia** has completed the development of the interfaces **WATER and EXTRACTOR** that run on the PC.

In **Steinar Hauan's group**, one new Ph.D. student (John Siirola, co-advised with Arthur Westerberg) joined the group in Jan 2001 while 2 students (Vikas Verma and Gogi Singh) have graduated with MSc degrees.

In his pursuit of feasibility analysis in reactive separation processes, Warren Hoffmaster has identified a region of additional reachability in azeotropic distillation where the residue curves have S-shaped local behavior. His current work is directed toward extreme conditions in cascade sections with simultaneous reaction, separation and extraction. Vikas Verma compared different collocation methods for reaction/separation processes and developed a system where the relevant model equations for a particular collocation configuration is derived automatically.

Gogi Singh took an initial look at the area of miniature process devices with special emphasis on novel unit operations arising from reaction, convection and mixing in small volumes. His thesis is a parametric concept study of model reduction and optimization of a flow-splitter with variable geometry. An effort in microscale gravimetric detection of biomolecules has been initiated with collaborators in BME, ECE and Biology.

Murni Ahmad has been working with Todd Przybycien on flexible design of biochemical processes. She is currently working on a modular optimization formulation of a 2-phase aqueous system for protein separation.

John Siirola joined the group in January to work with agent-based systems for distributed, asynchronous process design. The goal is to study how 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. A prototype Beowulf cluster for high performance parallel computing is in operation with stage #2 expected to be built in May.

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. A reexamination of problem formulation has led him to consider how to solve recursive dynamic programming problems having multiple objectives. Lifei passed his Ph.D. qualifier in January.

John Siirola is a new Ph.D. student whom both **Steinar Hauan** and **Art Westerberg** will co-direct. John will be working on the use of agent-based software concepts to analyze and optimize large process design and operation problems. He will use the large parallel computer cluster Steinar, David Sholl and Larry Biegler are creating in the department.

Erik Ydstie's research group continuous to work on process control and dynamic simulation of complex chemical process. We completed the work on *plant wide process control* 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. 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 and 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 have started a *process modeling* effort. The aim is to develop 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 develop a dynamic model of the their Silicon production process. This model will be used for control system design and *real time process optimization*.

The research group has re-initiated its interest in discrete event systems and we have started two projects in the area of *supply chain management*. One of these are carried out in c-operation 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 is developing and testing 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.

When applied to standard NLP test problems, this new Schur complement QP approach (called QPSchur) is about three times faster than QPKWIK. Moreover, it allows us to develop more flexible NLP strategies that deal with smaller reduced Hessians, better exploitation of sparsity and changing active sets. These features are similar to those in CONOPT but here we apply them in an infeasible path mode. 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 large dynamic optimization problems for NMPC and would like to know when barrier approaches 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
Student: Gregory Itle (Ph.D. student started Fall, 1998)

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 recently passed his Ph.D. proposal exam and is extending this approach 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 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.

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 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. He has also shown that trust region approaches, as developed by Byrd, Nocedal and coworkers, do not suffer from this difficulty. Because barrier methods have seen considerable activity in the optimization community, this example has attracted a lot of attention in the Math Programming community. Andreas has also 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 global convergence proof for his approach. Numerical testing 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

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. A paper that describes this work is listed below.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Students: **Arvind Raghunathan (Ph.D. started Fall, 1999)**
Maame Poku (Ph.D. started Fall, 2000)
Researcher: **Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Visitor: **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. A paper that describes this approach is listed below.

In order to allow large-scale applications of these dynamic optimization strategies, a software environment has been developed by Yi-dong Lang for Windows platforms. With this software Yi-dong has applied dynamic optimization to crystallization problems, batch reactors and open loop unstable systems. These are described by a DAE system and represent challenging nonlinear problems with interesting control profiles. As part of this project, Yi-dong has developed a prototype dynamic optimizer running under Windows and developed with Digital Visual FORTRAN. This package, called DynoPC has a GUI interface as well as a user-friendly front end. This is available to CAPD member companies on an ftp server. More recent work has included the implementation of Arturo's large-scale dynamic optimizer into the PC environment. 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.

Finally, Arvind Raghunathan has begun to work on dynamic optimization and the use of complementarity constraints in optimization problems. This allows us to build on the interior point efforts of Andreas, both in barrier methods and dynamic optimization. A key advantage is that complementarity constraints can be handled directly and simultaneously with interior point methods. This allows us to deal with problems that require conditional relations including phase equilibrium and disappearing units. Arvind has demonstrated this approach on the optimization of steady state distillation column models where trays can dry up (i.e., obtaining solutions below the minimum reflux). He is currently extending this approach to dynamic optimization problems with phase changes and other discontinuities due to switching. Also, Arvind is exploring the more general class of Mathematical Programs with Equilibrium Constraints (MPECs) which include the complementarity problems. A number of algorithms and problems are being tested in this class, including blending and equilibrium.

Dynamic Optimization Strategies using DAE Solvers

Students: **Ling Jiang (Ph.D. started Fall, 1999)**
Cong Xu (Ph.D. started Fall, 2000)
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. They have disadvantages for unstable systems encountered in reactive and control systems

but incorporate very efficient DAE integrators that are well-suited and well-tested for dynamic simulation. An additional bottleneck 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 has begun to work on this project. She has spent the summer at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, 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. This paves the way for dealing with much larger systems and extending them to optimization problems.

Cong Xu recently joined this project and will also be investigating optimization problems arising in fluid dynamics and transport phenomena.

Synthesis of Reactor Networks for Waste Minimization

Students: **William Rooney (Ph.D. started Fall, 1996)**
Visitor: **Shehzaad Kauchali (University of Witwatersrand, Fall, 2000)**

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 visited with us last fall to continue this interaction. The results of his visit led to a close synthesis of optimization and geometric methods for targeting attainable regions for reactor networks and an algorithmic approach for the construction of attainable regions for reactor networks. This approach is optimization based and deals with the development of lower dimensional projections that can be combined to obtain the full dimensional region. Since then, we have been developing prototype concepts for algorithmic generation of attainable regions using large linear programming formulations. Shehzaad Kauchali has joined us to continue this work. We intend to apply large-scale optimization to convex problems to generate these

regions. Preliminary results show that this approach is quite encouraging - and can be generalized to a number of multi-dimensional problems.

Moreover, Bill has 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. This approach 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. A paper that describes this approach is listed below. 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, Bill is considering 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 is developing strategies that deal with both types of these uncertainties in a flexibility framework. To solve problems of this type we are also applying 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 recently passed his Ph.D. proposal and is 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. These will be 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

Student: **Jennifer Jackson [Ph.D. , started Jan 99]**
Visitor: **Juan Reyes [postdoc, started June 00]**
Collaborator: **Jose Caballero [Asistant Prof., Univ. Alicante]**

New development: *Publication on reactive distillation optimization*

This project builds on the work of Hector Yeomans who developed a modeling framework for separation systems based on the State-Task Network (STN) and State Equipment Network (SEN) representations, and that are formulated with generalized disjunctive programming (GDP) models. A major aim of this work has been to develop tray by tray models for synthesis, including complex columns and azeotropic separation. The following three projects are under way:

Jennifer Jackson: Reactive Distillation
Jennifer has completed the first phase of her work on the optimal design of reactive distillation columns, We assume that in such a 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. The basic idea in Jennifer's model is to consider all trays as being conditional, except the condenser and reboiler. She also considered that 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 has developed nonlinear disjunctive programming model, which she solves with a variation of the logic-based outer-approximation method of Metin Turkay. She has 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. The significance of Jennifer's work is that it provides a fairly robust technique to optimizing reactive distillation problems. Also, her results show that single column feeds seem to be the exception rather than the rule. A copy of her manuscript is enclosed in this newsletter.

Juan Reyes: Liquid-Liquid extraction
Juan Reyes, who has returned to the University of Alicante in Spain, 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. Furthermore, Juan generalized the superstructure for the case of multiple feeds of the liquid that is to be extracted. Juan formulated the model as a disjunctive programming problem, also using the concept of conditional stages, and found significant improvement in the robustness of the calculations and a decrease in the likelihood of ending with suboptimal solutions when compared with an MINLP model. 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, which involved 10 boolean variables, 350 continuous variables and 547 constraints, was

solved in about 570 secs (Pentium II). Gabriela Garcia is currently implementing Juan's model as the interface EXRACTOR (see below).

Jose Caballero: Thermally linked columns.
Jose, who is also back in Spain at the University of Alicante, has been addressing 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.

Planning for Retrofit Design in Process Networks

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

Jennifer has only recently started to get back to this project, which was put on hold due to her involvement in the reactive distillation project. This project is concerned with developing high level optimization models for process modification that 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 is currently looking at two 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. Jennifer is also starting to embark on a project with Dow in which some of these models can be applied.

Algorithms for Nonlinear Disjunctive Programming

Students: **Sangbum Lee [Ph.D., started Jan 98]**
Research fellow: **Aldo Vecchietti [Ph.D., completed Aug 2000]**

New Development: *Publication on Global optimization algorithm for nonconvex disjunctive problems*

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:

$$\begin{aligned} \textit{Min} \quad & Z = \sum_i \sum_k c_{ik} + f(x) \\ \textit{st} \quad & g(x) \quad 0 \qquad \text{(GDP)} \\ & \bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(x) \leq 0 \\ c_{ik} = \gamma_{ik} \end{bmatrix} \qquad k \in SD \\ & (Y) = True \\ & x \in R^n, c \in R^m, Y \in \{true, false\}^m \end{aligned}$$

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 property Sanbum has proved rigorously in a revised version of the manuscript we had initially submitted. 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. In the last two months Sangbum has worked very hard in revising the proofs in a manuscript we submitted for publication to Mathematical Programming.

Sangbum has recently completed 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. This model assumes zero-wait policy and single-product campaigns 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. The manuscript describing this work is enclosed in this newsletter.

As described in the last newsletter, 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.

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. 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 feature of the new version 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. The alternative of solving the linear GDP with a special method we are also examining in collaboration with John Hooker, from GSIA.

Scheduling of Batch and Continuous Multiproduct Plants

Postdoctoral fellow: Iiro Harjunkoski (started September 1999]

New Development *Completion of steel plant scheduling and lower bound*

Iiro has undertaken two projects. The first has been to continue the work initiated by Vipul Jain for integrating CLP (Constrained Logic Programming) and MILP. Initially, Iiro applied the 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 that is implemented in STBS. 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 is 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 cuts for the MILP in this problem is much harder. Fortunately, Iiro found a way to generate these cuts using a graph representation of the schedule in which all paths of jobs in the last stage corresponding to tardy jobs are traced back to the first stage. 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. A copy of the manuscript describing this work is enclosed.

Iiro has largely completed the work on scheduling for steel manufacturing in collaboration with Kvaerner. This problem contains a large number of chemistry-, geometrical- and scheduling rules which makes already a problem containing 10 heats practically impossible to solve by MILP. The production is therefore highly sequence dependent. Certain properties of the problem, e.g. the fact that the products need to be grouped for the last operation motivate a decomposition of the problem. Iiro developed an effective solution 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: Completion of new branch and bound algorithms

Jayanth's current 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 initially restricted himself to batch flowshop scheduling problems.

Jayanth has developed a branch and bound procedure for flowshops with zero wait policy in which the key ideas in the new procedure are the following. First, for a fixed sequence Jayanth uses the analytical expression that was proposed by Karimi to simplify for computing the expected completion time. The idea is 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 that Jayanth exploited 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. The end result is a very effective branch and bound procedure that requires no explicit math programming model. 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. This branch and bound procedure Jayanth has extended to flowshops with UIS policy. He has also been able to extend it for continuous distribution functions. Rather than having to integrate analytically the corresponding pdfs he found that it is possible to use discretization schemes that provide excellent approximations, and in some cases exact answers. The idea relies on the fact that for univariate functions exact discrete approximations are possible for higher moments by the appropriate selection of discrete points that happen to correspond to roots of polynomials for Gaussian integration. As an example of the accuracy of this method, Jayanth solved a problem 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 been addressing recently the problem of parallel units with uncertain processing times, in which he has been able to exploit similar lower bounding properties, with which 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 is exploring the application of a genetic algorithm to optimize the schedule with his evaluation procedure.

Multiperiod Disjunctive Programming Algorithms

Student: **Susara van den Heever (Ph.D. started January 1997)**

New Developments: *Optimization of hydrogen supply pipelines*

Sarette's project deals with the solution of mixed-integer *nonlinear* multiperiod models. The major objective of her project has been to develop algorithms based on disjunctive programming and apply them to a number of planning problems. The major focus of application has been in the design and optimization of oilfield planning problems. Her most recent focus has been in the planning and operation of hydrogen pipelines.

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 has 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 has completed the work for 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).

In the last six months Sarette has 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 has 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 has used a rolling horizon strategy in which the planning model is solved successively with one period of the scheduling model. To address the issue of problem size she is currently exploring the use of Lagrangean decomposition.

Integration of Product Testing and Planning of Batch Manufacturing Facilities

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

New Developments: *Comprehensive MILP model for integration R&D and manufacturing*

The research project of Christos involves 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 consider 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. Also, Christos is almost finished writing up the manuscript describing this work.

Supply Chain Dynamics and Control

Student: **Edgar Perea (Ph.D. started January 1997)**

New development: *New dynamic model for analyzing effects in disturbances of demands*

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 is currently incorporating optimization in the form of model predictive control, 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 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 is exploring the use of a higher level static optimization model that determines the schedule and inventory levels, and is then implemented and verified with the dynamic model.

Software for MINLP Optimization in Design and Scheduling

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

New Developments: *New WATER and EXTRACTOR interfaces*

Gabriela has completed the interface OPT-WATER which is based on the work of Berta Galan for the design and synthesis of water treatment systems. This interface determines the optimal configuration of m treatment units given n streams that need to have several contaminants removed. The method accounts for all possibilities of mixing and splitting the streams. Gabriela has also essentially 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

Students: **Warren Hoffmaster (PhD, started Jan 2000)**
Vikas Verma (MSc, graduated Dec 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 is working to identify the proper limiting conditions in processes where reaction and separation takes place in the same piece of physical equipment. The fundamental approach is to view design of these devices as configuration of a cascade sections, each of which has their own limiting and optimal behavior in composition space. In our recent theory of generalized difference points, we have shown how the equations governing the profiles of such cascades emerge as a sequence of normalized linear combinations. Warren has just completed a paper that combines bifurcation/continuation software with geometric arguments and identified a set of reachable compositions for azeotropic distillation systems found outside the region enclosed by total and minimum reflux curves. Using his own generic cascade implementations, he has also validated the basic geometric variants in cascades with simultaneous reaction and separation. The next step is to identify the reactive pinch point curves and extend the methods to extractive sections. Vikas' goal was to prepare ground for performing comparative studies of sequential versus simultaneous reactive separation processes. In order was investigated. A key results is that performance of these methods depends critically on the choice of collocation elements and points as well as the exact placement of polynomial roots. Unfortunately, the model equations are specific to each such collocation configuration, forcing the models to be rewritten for each case independently The result of Vikas' work is a modular approach in which the relevant collocation equations may be derived automatically for any choice of polynomial types and roots.

Microscale Process Design

Student: **Gogi Singh (MSc, graduated Feb 2001)**

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 microgravimetric 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

Gogi Singh has just completed his MSc thesis on numerical simulation of flow patterns for various geometries representing standard "unit operations" in chip-based system with special focus on channels, wells, splitters and mixers. As reported in the literature, these systems are characterized by laminar flow and the assumption of fully developed Poiseuille flow is a reasonable one as long as the downstream distance to geometric abnormalities is more than approximately 4 times the channel width. Further, care must be exercised when determining the input/output specifications for coupled unit operations as only a subset of them lead to a unique solution. Gogi first developed a system for conducting semi-automatic case studies in pressure driven flow splitters that generate reduced order model representations of the underlying PDEs. Next, he performed
discrete optimization of the splitter shape with pressure dependent performance of reactor systems at the end of each pipe. 3-D models of microreactors are currently in development using similar techniques.

For molecular detection, Kaigham Gabriel's group has created four prototype polymer membranes with embedded electrodes on a standard silicon chip. In the months to come, we will be testing the functionalization chemistry on surfaces with and without gold cover as well as designing a detection chamber in acrylic plastic through the use of a special laser engraving "printer".

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 currently studies the design of protein separation systems by 2-phase aqueous solutions of poly-ethylene glycol (PEG) and dextran. Key variables in addition to normal process specifications include molecular weight of the organic polymer and the concentration of salt added to the solution. Murni is working on a modular implementation of thermodynamic methods that will fit into an optimization framework.

Agent-Based, Asynchronous Process Design

Student: John Siirola (Ph.D., started Jan 2001)

Background

Co-advised by Arthur 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.

Progress

John has also started implementing the basic proof-of-concept modules for distributed task coordination and database operations.

We have a running 7-cpu prototype of a Beowulf computer cluster based on a customized version of RedHat Linux and built from generic components. Care has been taken to build homogeneous environment with a scalable infrastructure and easy installation and maintenance. An expansion plan was recently funded by the National Science Foundation; the 2nd stage will be operational in May and consist of approximately 30 computer nodes with dual 1ghz Pentium III cpu's and at least 1 gb of physical memory. Stage 3 is expected to take place late in the year.

Gary Powers' Group

Process Risk Assessment Using Symbolic Model Checking

Students: Dan Margolis and Dan Milam

Dan Margolis and Dan Milam presented their Ph.D. proposals in February and are now scheduling the research and development plans they presented.

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

Dan Margolis is working on the operating procedures that describe the logic of how operators and maintenance workers interact with the process. He is building an operating procedure language that can be interpreted into the discrete event language currently used in Symbolic Model Checking. He is also considering how the synthesis of operating procedures could be guided by the Model Checking approach. He is building on the research of Dr. Bob Fusillo and Dr. Tom Teague both of whom worked on the operating procedure synthesis problem. Dan Margolis is applying his operating procedure approach to the synthesis and verification of procedures for a complex solids forming process that involves 5 operators and maintenance personnel interacting with over 12 pieces of major equipment and a control system made up of 5 PLCs and one supervisory computer.

Dan Milam is generating a library of modular models that can be interconnected to generate system models for use by the Symbolic Model Verification program. He is developing methods for the synthesis of discrete event hybrid system models, which are derived from the specifications, which are to be checked on the process. The coverage of these models (do they include 'all' the important behaviors) is being investigated both theoretically and experimentally. Mr. Milam's work is using the research results from Dr. Scott Probst and Dr. Adam Turk. Mr. Milam is also studying the solids forming process mentioned above and is building methods for interpreting the PLC and C++ code into SMV models to be coupled to logic models of the equipment. He will also work on combining the control, equipment and operating procedure models into one systems model.

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 is trying out 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 showed that one can partition a problem into a nonstationary first say ten years and then a stationary problem from then on. One can first 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.

Recent progress: Lifei has been examining reformulating of the stochastic problem he wishes to solve. It has become apparent that these problems 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 is in business in 10 years and prospering. 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 it projected a negative expected future worth along any path and if it ends up on that path, it might elect to shut down. He is now asking how to handle solving multi-objective stochastic optimization problems. It is far from straight forward. But with multiple objectives, one can express more realistic problems.

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

John is just starting his project. He will be looking at how to pose and solve very large design and operation problems where

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

while assuming 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 will be 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 particular 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?

The first question John will be trying to quantify is the impact of this solution sharing on the time to solve.

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. One will be from Hangzhou in China and should be here in July. His interest is in modeling. The other will be from Argentina and has an interest in information technology.

Product Design Course: Among his current activities, he 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 is developing a new algorithm for adaptive control. The method incorporates a method that will stop 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 is currently working at PPG to test her ideas in an industrial environment. She 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 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 retains its performance so that optimal performance is achieved at each operating point.

Jennifer is now developing 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 will be tested on industrial scale processes next year.

Stability and Control of Process Networks

Students: Duncan Coffey (Graduated February 2001)
Vianey Garcia-Osorio

Duncan Coffey works on modeling and stability analysis of process networks. A process network is an interconnection of simpler processes, the most basic being the elemental operations of heat-transfer, chemical reaction, mixing, and phase-separation. Duncan has developed a stability theory for networks of such processes, and he has shown that the network is stable if each element is passive and certain interconnection and boundary conditions are satisfied. The underlying theory is based on thermodynamics (the second law in the Clausius-Planck formulation) and the passivity theory of nonlinear control. Duncan has used the theory to show that multi-component distillation is open loop stable when the boundary conditions are suitably chosen. He has developed control systems for distillation that control to given setpoints. The latter work was carried out in cooperation with Professor Sten Bay Jorgensen at DTH in Copenhagen.

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.

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Y-01-04
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