CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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GENERAL NEWS

Steinar Hauan has been selected for the 2002 Ted Peterson Student Award of the Computing and Systems Technology Division of AIChE. This award is given for published work in process systems engineering, while pursuing graduate studies in chemical engineering. Steinar was quoted for his papers in the area of reactive distillation. He will be receiving this award at the Annual Meeting in Indianapolis.

Ignacio Grossmann was awarded in May, an honorary doctorate from Abo Akademi in Finland. Ignacio was also found by ISI (Institute Scientific Information) to be one of the top 15 most cited authors in papers that are classified as belonging to the computer science discipline.

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

Dirk Brusis from the Technical University in Munich and Jehoon Song from KAIST joined Ignacio's group. Dirk will stay for 3 months and work on MINLP models for complex distillation columns. Jehoon will stay for 6 months and work in the area of supply chain optimization. Martin Houze returned to France after completing the project with TOTALFINAELF on catalyst deactivation.

Edgar Perea, who worked with Erik and Ignacio in the area of dynamics and optimization of supply chains, successfully defended his Ph.D. thesis, and accepted a position with PEMEX in Mexico. Sangbum Lee, who worked with Ignacio in the area of Generalized Disjunctive Programming, successfully defended his Ph.D. thesis in May and is currently doing a postdoc in Ignacio's group.

Vanesa de la Torre from PLAPIQUI, Bahia Blanca joined Larry's group. She will be working on load following optimization for PSA systems. Ricardo Perez recently returned to Pontifical University of Chile and Daeho Ko recently returned to Yonsei University in Korea.

FOCAPO 2003

Ignacio is co-chairing together with Conor McDonald the FOCAPO (Foundations of Computer Aided Process Operations) 2003 Meeting that will take place on January 12-15, 2003, in Coral Springs, Florida. The theme of the meeting is "A View to the Future Integration of R&D, Manufacturing and the Global Supply Chain." Information about this meeting can be found in http://www.cheme.cmu.edu/focapo. We have been able to put together an exciting program, and expect to attract many industrial practitioners. Registration and an update of the program are now available at the website.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* was offered on June 20-26, 2002. We were very pleased with the outcome of this course. We had 13 attendees from around the world, both from industry and academia. Also, the course has been extensively revised and includes the following modules:

a) Conceptual Design - taught on Thursday and Friday (June 20-21), with focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.

b) Optimization - taught on Saturday and Monday (June 22 and 24), with focus on modeling and algorithms for nonlinear programming and mixed integer programming including disjunctive programming and applications to process optimization.

c) Process Operations - taught on Tuesday and Wednesday (June 25-26), with focus on differential/algebraic models for real time optimization and parameter estimation, and on mixed-integer programming models for process scheduling and supply chain management.

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

WEBSITES/PROCESS SYSTEMS DIRECTORY

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

We would appreciate receiving feedback from our member companies of our CAPD website, **http://www.cheme.cmu.edu/research/capd/.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Other websites of interest are Ignacio's http://egon.cheme.cmu.edu, and Larry's http://dynopt.cheme.cmu.edu. Also, the department maintains the website of CEPAC (Chemical Engineering Pan American Collaboration), the organization that has been formed to promote collaboration between the US and Argentina, Brazil and Chile. You can find in **http://cepac.cheme.cmu.edu** a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada and Chile. Mexico's will be added soon.

CAPD REPORT SERIES

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

EXECUTIVE SUMMARY

Highlights of **Larry Biegler's group** include further development of the reduced Hessian SQP (rSQP) strategy along several directions. The FORTRAN version of the rSQP strategy has been used for optimization of black box units including PDE based models involving convection and diffusion. Examples of this include CVD reactors (**Greg Itle**), PSA systems (**Ling Jiang**) as well as other fluid flow systems (**Cong Xu**). **Andreas Waechter**, who recently completed his Ph.D., has developed a novel and very efficient barrier (interior point) NLP method, called IPOPT, based on many of these SQP concepts. This has been used to solve problems that incorporate a number of specialized decomposition strategies and for a wide variety of applications with up to 2 million variables. IPOPT is available under an Open Source software license; more information on downloading and distribution is given below. The IPOPT strategy has spawned exciting applications to challenging problems in process engineering. First, **Arvind Raghunathan** is extending the IPOPT algorithm to deal with Mathematical Programs with Equilibrium

Constraints (MPECs); these arise frequently in separations and hybrid systems. In addition, **Maame Poku** is applying IPOPT, its extensions to MPECs, and its AMPL interface, to blending problems. Finally, **Roscoe Bartlett,** who completed his PhD in August, has developed a comprehensive suite of optimization routines called rSQP++. Written in C++ with numerical routines in FORTRAN, this suite was demonstrated on a wide variety of optimization applications. rSQP++ will be available under Open Source software licenses and more information on distribution will be in the next newsletter. In a new project, **Carl Laird** will be extending the work of Roscoe by incorporating the IPOPT algorithm as well as large-scale extensions into rSQP++.

In addition, **Yi-dong Lang** has developed a user-friendly version of dynamic optimization methods. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called DynoPC, runs under Windows with a GUI interface. It has been distributed to several CAPD members and can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package has been enhanced further by incorporating the ESO CAPE-OPEN modeling standards currently used in gProms. In a parallel effort, we are working with researchers **Tobias Jockenhoevel** from the Technical University of Berlin on the OCC package, which incorporates these dynamic optimization strategies using MATLAB interfaces. In a new project, **Shivakumar Kameswaran** will be expanding the work on dynamic real-time optimization using OCOMA as well as deriving theoretical properties of this approach. In addition, three visitors, **Daeho Ko, Ricardo Perez**, and **Vanesa de la Torre** are working on applications of dynamic optimization of large scale systems. Daeho is working on PSA optimization for CO2 capture, Ricardo is addressing the optimization of cellular systems and Vanesa is developing optimization strategies for load following of PSA systems. 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. In addition, he has also developed a robust NLP algorithm for this class of problems.

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

In the area of optimization **Nicolas Sawaya** has been investigating the use of cutting plane techniques for solving Generalized Disjunctive Programming problems in which the convex hull transformation may yield a very large problem, and exhibit poor relaxation. He is testing these ideas with the stock cutting problem. **Sangbum Lee**, has continued work on a very challenging project with BP for structural flowsheet optimization of olefins plants in which simultaneous optimization and heat integration is performed. **Aldo Vecchietti**, has completed the version of LOGMIP that can transform disjunctive problems with linear constraints into MILP problems with big-M constraints or convex hull reformulations.

In the area of process synthesis **Mariana Barttfeld** has developed a new solution strategy based on thermodynamic initialization and disjunctive programming for the synthesis of complex column configurations that rely on tray-by-tray models. **Dirk Brusis** has written a short note describing the use of external functions in GAMS for calculation of thermodynamic properties in GAMS for distillation optimization. **Jose Caballero** in Alicante has developed a systematic method based on propositional logic for generating thermodynamically equivalent superstructures for thermally coupled columns. In both cases we enclose a manuscript relevant to that project.

In the area of planning and scheduling **Jennifer Jackson** has completed the work on a new temporal decomposition of a multisite multiperiod optimization planning model using Lagrangian decomposition, and found it to be superior to spatial decomposition. **Jehoon Song** completed a multiperiod MILP model for the optimization of supply chains of crude oil systems, and for which he developed a rolling horizon strategy with aggregation. **Vikas Goel** has developed an approximation algorithm for the optimization of oilfields with uncertain sizes and productivities. **Jayanth Balasubramanian** has considered short-term batch scheduling problems with uncertain demands for which he is exploring a novel multistage-stage programming strategy that relies on a shrinking horizon solution strategy that involves solving smaller MILPs. **Christos Maravelias** has completed the work on a new method based on implied precedences and

decomposition for the resource constrained scheduling problem for the testing in new product development. He also has developed a new continuous time MILP model for STN short term scheduling, which aside from being computationally effective, can be shown to be rigorous compared to previous work. **Gabriela Garcia** has completed the first version of the web-based system for interfaces and in which GAMS is automatically invoked.

Steinar Hauan's Group

In his work on design algorithms for reactive separation processes, Warren Hoffmaster applies a decomposition technique to isolate the effect of internal reaction distribution. Inside an arbitrary separation cascade, the structure of feasible designs depends on the local and regional interactions between reaction and phase behavior. A subset of the alternatives may now be identified and solved based on a single flash calculation, but others still require a convex hull approximation of the reachable compositions. The approach is being validated against a set of literature examples.

John Siirola (co-advised by Art Westerberg) has expanded his agent system for solution of large-scale engineering design problems into the multi-objective domain. A modular C++ implementation is currently operational on our Beowulf cluster, and agents for tracking and expanding a non-convex front of pareto optimal solution have been added.

Anton Pfeiffer is working on system level design models for electrophoretic separation on a microchip. A 2-D component simulation model has been developed in Matlab to predict the separation and dispersion of analyte bands traveling through serpentine turns. The model is purely algebraic, but closely matches results obtained by finite element simulations. Simple (NLP) optimization capabilities have been added for a pre-defined channel topology; the next step is to extend the model to variable (MIP) topologies and incorporate the effect of area and layout constraints.

The goal of Michael Bartkovsky's project (co-advised by Todd Przybycien) is to create a gravimetric detector by surface functionalization of a polymer membrane on a chip. Device responses and power spectra are being assessed by eigenvalue (finite element) solutions of the wave equation with uneven mass distribution. The next steps are to incorporate the effects of damping and solution interactions and to calibrate the membrane stiffness from experimental results. Parallel work on the surface chemistry and solution properties are being carried out with proteins on a QCM setup in Todd's lab.

Our Beowulf cluster will be expanded in early September by the addition of a dedicated database server and 24 new P4 Xeon machines that should approximately double the capacity.

Professor Gary Powers' Group

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

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

Dan Milam is generating a library of modular models that can be interconnected to generate system models for use by the Symbolic Model Verification program. He is developing methods for the synthesis of discrete event hybrid system models, which are derived from the specifications, which are to be checked on

the process. The coverage of these models (do they include 'all' the important behaviors) is being investigated both theoretically and experimentally. Mr. Milam's work is using the research results from Dr. Scott Probst and Dr. Adam Turk. He is currently applying this approach to a computer controlled casting system.

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

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

In **Art Westerberg's group**, **Lifei Cheng** continues his work to create a simulation/ optimization/ design/ operation capability for stochastic models that describe the long-term future behavior of a process. He continues his work to develop approaches to allow him to solve larger problems of this type. He is spending two months this summer at Exxon/Mobil working on related problems.

John Siirola, working with **Steinar Hauan** and **Art Westerberg**, is developing agents and testing them to develop the trade-off surface (Pareto front) for multiobjective problems.

A postdoc with **Art Westerberg**, **Gabriela Mannarino**, from Santa Fe, Argentina, is developing software to allow users of n-dim to add different views and operations to n-dim.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

rSQP++: **A Framework for Large Scale Optimization Strategies**

Student: **Roscoe Bartlett (Ph.D. student completed August, 2001)**
Carl Laird (Ph.D. started Fall, 2001)

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

In addition, Roscoe has developed rSQP methods based on the application of Schur complements for the active set strategy in the QP. This approach has been very successful for the SOCS code at Boeing. Unlike the QPKWIK algorithm, the application of Schur complements allows us to directly exploit the structure of the entire KKT matrix at the linear algebra level. When applied to standard NLP test problems, this new Schur complement QP approach (called QPSchur) is at least three times faster than QPKWIK and about an order of magnitude faster than QPOPT on unstructured problems. As a stand-alone QP package, QPSchur has been compared against QPKWIK, QPOPT, LOQO and the MATLAB QP code on large-scale problems in Model Predictive Control (MPC). This problem, with up to 600 inputs was based on the cross-directional control of a paper machine. For this test problem, QPSchur was at least an order of magnitude faster than

any of the competing codes. Moreover, with the application of QPSchur we were able to demonstrate that the on-line solution of MPC controllers based on quadratic programming is indeed feasible for these challenging processes.

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. Moreover, rSQP++ allows us to develop much more flexible NLP strategies that deal with structured Hessians, better exploitation of sparsity and changing active sets. Finally, the resulting strategy fits well with the object oriented construction of the program and also serves as a nice complement to the barrier strategies discussed below. In fact, our goal is to identify problems where different problem classes can exploit various SQP options. For this purpose, we have considered linear model predictive control problems and large dynamic optimization problems for NMPC. In the former case, Roscoe showed that QPSchur is very efficient on these problems, particularly if the number of inputs is large. For the latter case, we are interested in knowing when barrier approaches (see below) are favored over active set strategies.

Carl Laird has recently joined the group and will be working on extensions to rSQP++. In particular, he has augmented rSQP++ features to include the filter line search from Andreas Waechter along with a barrier method for NLPs. Combining this barrier approach with the flexibility of rSQP++ will allow us to address much larger optimization problems. In particular, this activity will allow us to address multiperiod problems for design under uncertainty as well as large-scale dynamic optimization problems within rSQP++.

Large-Scale Optimization for Partial Differential Equation Models

Students: **Gregory Itle (Ph.D. student started Fall, 1998)**
Cong Xu (Ph.D. student started Fall, 2000, joint with Prof. M. S. Jhon)

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

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

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

Barrier (Interior Point) Methods for Nonlinear Programming

Students: **Andreas Waechter (Ph.D. completed January, 2002)**

Andreas recently completed his Ph.D. and has taken a postdoctoral position at IBM Watson. This project considers the development of an efficient strategy for solving nonlinear programs using interior point (IP) methods. This approach works either in the full space or can take advantage of the particular rSQP decomposition strategies (choices of Z and Y) that we have developed in previous work. The advantage of this approach is that it solves the nonlinear problem directly without first exploring the solution of the QP subproblem. In this way we avoid the overhead in solving highly constrained QPs, as these have the same level of combinatorial complexity as the original NLP problem.

Andreas developed and tested a number of variations to this approach that include the use of line search approaches, decoupling the barrier terms from the reduced Hessian approximation and options for both primal and primal-dual barrier terms. Along these lines, Andreas has discovered that Newton-based IP methods that are applied directly to NLPs can experience convergence failures. These failures are analogous to infeasible QPs that can be encountered in SQP but are much more subtle because the cause cannot be detected easily. In particular, Andreas has developed a counter-example that illustrates this problem, and has also developed a through analysis of this difficulty. A reprint of the paper that discusses this phenomenon is listed below. In addition, Andreas has developed an improved line search algorithm that is based on a recently developed *filter* approach. This approach overcomes this convergence difficulty and Andreas has completed a rigorous convergence analysis of his approach. Numerical testing on over 700 test problems has also shown some significant performance improvements over other barrier algorithms. Major features of this approach are:

- an implementation that allows either full space or reduced space options for the barrier NLP. In particular, the reduced space option has been tailored to the structure of DAEs solved with collocation on finite elements.
- a filter line search approach that replaces the classical merit function for line searches
- a preconditioned conjugate solver for the null space step that replaces quasi-Newton updating and uses true second order information instead of just quasi-Newton information.

To test these ideas, a FORTRAN code has been implemented for the solution of dynamic optimization problems; problems with over two million variables have been solved in a few hours of CPU time on an 700 MHz computer. Moreover, this approach has been linked to a number of packages including DynoPC, OCOMA and AMPL. Finally, an open source license is being prepared for this code. Our first version of this code can be downloaded from: http://www.coin-or.org

Mathematical Programs with Equilibrium Constraints (MPECS)

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

MPECs represent an exciting new field in mathematical programming. While applications of MPECs have long been recognized in game theory, transportation planning, economics and engineering design, little work has been done in developing efficient algorithms for their solution In process engineering, these problems stem from bilevel and multilevel optimization problems as well as optimization of hybrid (discrete and continuous) systems. Included in this class are optimization problems with phase equilibrium constraints, as in equilibrium stage processes.

The MPEC problem is essentially a nonlinear programming problem augmented by complementarity conditions. The addition of these conditions leads to a violation of convergence assumptions for most nonlinear programming algorithms (e.g., linear independence of the constraint gradients) and can cause these algorithms to fail. On the other hand, the barrier method described above has a straightforward extension to these problems. As a result, complementarity constraints can be incorporated with little additional cost in the algorithm. In fact, all of the features that contribute to the efficient performance of IPOPT can be invoked directly for the solution of the MPEC problems. The resulting algorithm based on IPOPT has been developed further and refined for a number of challenging dynamic optimization applications in process engineering. Preliminary work in this area includes the following:

Arvind Raghunathan has incorporated the MPEC formulation into the IPOPT code along with algorithmic modifications to treat the complementarity constraints more efficiently. This code has been interfaced to the AMPL modeling system and has been tested on a set of library MPEC problems. Preliminary results show that this implementation compares well against competing barrier algorithms such as LOQO. Arvind tested this approach on a number of process optimization problems with phase equilibrium constraints. These include distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages. Preliminary results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies. Arvind has also dealt with modeling conditional relationships using complementarity conditions instead of binary decision variables. While this leads to nonconvex NLPs, the solution of these MPEC problems can lead to satisfactory solutions with less computational effort than in solving MINLPs.

Maame Poku has applied IPOPT with the AMPL interface to deal with nonlinear planning and blending problems. These problems have a large number of superbasic variables (degrees of freedom). As a result, reduced space NLP algorithms (like rSQP, MINOS, CONOPT and SNOPT) do not work well. Preliminary results show that the full-space version of IPOPT works quite well on these problems. A preprint that provides results of this strategy is listed below.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Students:	**Arvind Raghunathan (Ph.D. started Fall, 1999)**
Researcher:	**Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Visitors:	**Tobias Jockenhoevel (Technical University of Berlin)**
	Prof. Ricardo Perez (Pontifical University of 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 preprint that extends this work to cryogenic systems is listed below.

For these large-scale optimization algorithms, it is essential to develop modeling environments that allow an efficient and convenient formulation of DAE models for dynamic optimization. A review of our efforts in this area along with a summary of new results is listed below. For this task, we are building on several international collaborations, and are leveraging work done with existing and emerging modeling concepts.

First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called DynoPC. Written for Windows 2000 with a Visual Basic user interface and with a heavy integration of graphical, simulation and automatic differentiation tools, this software package was recently updated to incorporate ADOL-C and our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from http://coin-or.org Future developments of DynoPC will be augmented in collaboration with Prof. Marquardt's group at the Technical University at Aachen (RWTH). Here we are incorporating ESO interfaces, developed by the gProms group that are compliant with recently developed CAPE-Open protocols. This will lead to an interface that will be compatible with a number of existing process models and modeling environments.

Second, we are interfacing and benchmarking our algorithms to other popular modeling environments. In collaboration with Prof. Tsatsaronis at the Technical University of Berlin, Tobias and Yuen are incorporating the IPOPT algorithm within OCC (see http://www.optcontrolcentre.com), a MATLAB-based package for on-line optimization, system identification, off-line steady state and dynamic optimization and process monitoring. In particular, this package incorporates a number of discretization strategies (Gauss and Radau collocation, implicit Euler and BDF formulas) as well as the full algorithmic, graphical and modeling capabilities of MATLAB. With this collaboration we plan to exploit the benefits of a MATLAB interface for dynamic optimization. Our future work will enhance the formulation and algorithmic capabilities of MATLAB-based packages like OCC and to combine them with our efforts in the development of DynoPC.

Finally, Prof. Ricardo Perez is exploring the use of dynamic optimization for biological systems with Arvind Raghunathan. Together they have explored the data reconciliation of metabolic flux models in yeast and E. coli systems. The optimization formulation takes the form of dynamic optimization problems with embedded LPs. This problem has been treated with an MPEC formulation and has been solved using a variation of IPOPT. Results of this approach will be described in the next newsletter.

Optimization of Pressure Swing Adsorption Systems

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

In tandem with the above project, we are also developing more direct sequential strategies for the solution of dynamic optimization problems. These approaches are better known and have seen a lot of previous development. An important aspect to these sequential strategies is obtaining sensitivities from the dynamic model efficiently. Fortunately, recent projects by Barton at MIT, Petzold at UC-Santa Barbara, and researchers at the Max Planck Institute have led to excellent software implementations that calculate sensitivities efficiently from large DAE process models. Also, these sequential approaches take advantage of 'off-the-shelf' solvers and do not require a heavy research investment as with simultaneous methods. As a result, we are embarking on large-scale dynamic optimization projects that combine our large-scale rSQP tools with efficient DAE solvers and sensitivity codes.

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

models and implementations for the optimization of comprehensive, detailed PSA systems. Up to now, no satisfactory optimization strategies have been developed that can deal with these models. Ling Jiang has generated a number of interesting results for this project. She is spending her summers at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, and automatic differentiation codes, like ADIFOR, to adsorption bed models created from the method of lines. In particular, she concentrated on developing detailed PSA bed models with hyperbolic and parabolic components that require special mass conserving discretization strategies to convert them to DAEs. Termed flux limiters, these discretizations allow the accurate tracking of steep fronts and discontinuities that frequently arise in PSA systems. Ling has successfully simulated and optimized cyclic steady state conditions for two PSA units, using Newton-type and tailored rSQP solvers. From this point she has demonstrated a framework that includes constrained simulation problems and design optimization problems on a number of PSA examples. *Preliminary results of her work show that this optimization strategy can reduced the power requirements for PSA systems by about 15% and the computational cost is an order of magnitude less that with conventional case study approaches* .More recently, she has implemented this approach to run in parallel on our Beowulf cluster; this leads to tremendous speedups in PSA optimization, as the sensitivity equations are trivial to parallelize. Results of this parallelization will be described in the next newsletter. In addition, Vanesa de la Torre recently joined the group and is developing optimization models for PSA systems that address load following approaches induced by changes in product demand.

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

Data Reconciliation for Steady State and Dynamic Processes

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

Currently, Nikhil is extending data reconciliation and parameter estimation strategies to both steady state and dynamic processes. He is applying statistical tools to determine steady state conditions, classify measurements and observed model variables, detect data outliers and estimate model parameters. In particular, Nikhil is investigating more general classes of M-estimators for gross error detection within a simultaneous optimization framework. In particular, Nikhil will apply these approaches to an industrial project on carbothermic processes for silicon metal refining and casting. For these processes, dynamic furnace models are being developed (with Martin Ruszkowski and Prof. Erik Ydstie) and efficient strategies are needed for data reconciliation and parameter estimation for the existing process.

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

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

being incorporated within a large scale SQP framework as well to take advantage of rapid convergence. A paper that describes this work is listed below.

Finally, Shivakumar Kameswaran has recently joined the group and is working on system identification and parameter estimation for oilfield applications. Using IPOPT and OCC as a dynamic optimization tool he is studying parameter estimation for distributed parameter systems that are potentially ill-conditioned. In future, Nikhil's large scale NLP strategies will also be applied to these problem types.

Ignacio Grossmann's Group

Algorithms for Nonlinear Disjunctive Programming (ALMOST DONE)

Student:	**Nicolas Sawaya [Ph.D., started Jan02]**
Postdoctoral fellow:	**Sangbum Lee [started May 2002]**
Research fellow:	**Aldo Vecchietti [Ph.D., completed Aug 2000]**
New Developments:	*Cutting planes for GDP problems with poor relaxation*
	Mass and heat optimization for a superstructure of olefins process.
	LOGMIP completed for linear disjunctive constraints

Nicolas Sawaya

The overall objective of Nick's project is to develop novel solution methods for nonlinear generalized disjunctive programs (GDP). Sangbum laid the foundation for obtaining relaxations in convex nonlinear GDP problems through the convex hull of each disjunction. There are two major issues that arise in the continuous relaxation based on the convex hull for linear or nonlinear problems: (a) the corresponding formulations may lead to a problem of large size due to the disaggregation of variables; (b) the corresponding relaxation may produce a lower bound similar or equal to the one obtained from the big-M reformulation of the GDP. The second issue was studied by Aldo and Sangbum, who concluded that the nature of the disjunctions (proper or improper) when projected in the continuous space can indicate the degree to which there might be a difference between the convex hull and big-M relaxations. A major objective in Nic's work is to first investigate whether one can theoretically determine if the convex hull relaxation is strictly tighter than the big-M reformulation, and second develop effective solution methods of GDP problems that may exhibit poor relaxations.

In order to address the above issues the first step in Nick's work has been to investigate how to project the higher dimensional equations of the convex hull into the original space of discrete and continuous variables. The basic idea relies on analytically solving for the parametric Lagrangian from the minmax feasibility problem applied to the convex hull constraints. While theoretically this approach provides a framework for the unambiguous comparison of the convex hull and big-M relaxation, it is very difficult tom implement for large-scale problems. Therefore, there is motivation for an effective numerical procedure that can at least bound the comparison of the relaxations. The procedure that Nic has used is one that relies on the derivation of cutting planes. This is accomplished as follows. We first solve the big-M relaxation. Next, we formulate and solve a separation problem in which we minimize the difference between any feasible point in the convex hull relaxation and the solution of the big-M problem. Here we can use the 1, 2 or infinity norm, with the first and last leading to linear objectives. If the difference in the separation problem is small or even zero this is a clear indication that the both the big-M and the convex hull relaxations are essentially identical. If, on the other hand, the difference is not small this not only tells that the convex hull formulation is tighter, but one can derive a cutting plane, which for the linear case corresponds to a facet of the convex hull.

Nic has examined the application of the cutting plane procedure to the 2-dimensional stock cutting problem. This is a well-known and surprisingly difficult combinatorial problem that consists of finding the shortest length of a rectangle with fixed width that can accommodate a given set of smaller rectangles with fixed dimensions. This problem can be formulated in a compact way as a GDP problem. In a small problem involving 4 rectangles, Nic found that the big-M reformulation required about 100 nodes in the branch and bound search, while the convex hull formulation required only about 25, although both gave the same LP relaxation at the root node. The big-M with one cutting plane required only about 30 nodes, with the

advantage that it involves fewer constraints and variables. Nick is in the process of testing these ideas in larger problem in preparation for his Ph.D. qualifying exam.

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

Sangbum Lee

After a successful Ph.D. defense in which Sangbum impressed the committee with all the work he accomplished (e.g. derivation equations of nonlinear convex hull of GDP, disjunctive branch and bound search, two-level global optimization of GDP and bilinear process networks, LP model for identifying alternate optima in metabolic networks, synthesis of Eastman's monomer process), he has taken a postdoc position in Ignacio's group. Sangbum has been working on a special project in collaboration with BP (Jeff Logsdon and Mike Foral) that deals with the superstructure optimization of an olefins plant. Sangbum has developed a superstructure for the separation section considering several technologies for the various separation tasks (e.g. distillation, absorption, cryogenic, membranes, etc.). He has also developed simplified models that can accommodate both sharp and non-sharp splits, and heat integration. A novel aspect of the latter has been to use a continuous representation of the cost of utilities as a function of the temperature, which reduces the number of discrete variables that are needed. The GDP was transformed into an MINLP, which is of the order of 2000 0-1 variables, and 12,00 continuous variables and 25,000, and solves in about 2 hours with DICOPT on a Pentium-III. The major effort in the recent months has been to improve the accuracy of the model, which is being tested with the ASPEN simulator. So far the model has been able to predict significant reductions in cost, particularly in the energy use.

Aldo Vecchietti: LOGMIP and modeling issues

The main thrust of the work by Aldo has been the developments of LOGMIP, as well as the analysis of alternative models for disjunctive programming, which was performed in collaboration with Sangbum. Aldo and his students at INGAR in Argentina are developing the LOGMIP code, which is as an extension of the GAMS modeling language for posing logic/disjunctive problems. The main features of LOGMIP are several language constructs in order to concisely formulate GDP problems. The syntax that he developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. An interesting related development has also been to show that logic constructs that are commonly used in Constrained Logic Programming (CLP), such as implications for constraints (eg g(x) 0 => f(x) 0) can be systematically converted in the form of disjunctions. As for the propositional logic, we have decided to develop special constructs such as ASSIGN, ATLEAST, ATMOST, IMPLIES, etc. to facilitate the specification of global logic constraints. For the general case, the propositional logic can be 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 has just completed a first version for the implementation of the convex hull relaxation and big-M transformation for linear problems. He has implemented this in the IDE version of GAMS. Aldo successfully tested the code with small and medium sized problems that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. Aldo has also automated the logic-based OA algorithm, which is suitable for nonlinear GDP process network problems. An example of part of the input in GAMS that can be accomplished with LOGMIP is shown below:

```
DISJUNCTION D1,D2;

D1 IS
IF Y('1') THEN
      EQUAT1;
      EQUAT2;
ELSIF Y('2') THEN
      EQUAT3;
      EQUAT4;
ENDIF;

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

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

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: *Comparative study between MINLP and GDP models for distillation design*
Logic constraints for thermally integrated columns
Use of external GAMS functions for thermodynamic calculations

Students: **Mariana Barttfeld (Ph.D. INGAR), Jennifer Jackson [Ph.D. , started Jan 99]**
Collaborators: **Dirk Brusis (Ph.D. student Technical University of Munich),**
Jose Caballero [Assistant Prof., Univ. Alicante]

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

Mariana Barttfeld
Mariana is staying with Ignacio's group for one year in a collaboration with Prof. Pio Aguirre from INGAR in Argentina. She first performed a comprehensive comparison between MINLP and GDP models for optimal design of distillation columns in which tray-by-tray models are used. For the MINLP models she considered superstructures in which, (a) the feed is fixed and the reflux and reboil returns to a number of potential trays, (b) the reboil is fixed and feed is introduced at all potential trays and the reflux returns to a number of potential trays, (c) like case (b) except the role of reflux and reboil is exchanged. For the GDP model she has considered both the case of fixed reflux, feed and reboiler trays, and all other as conditional trays, and the case where the feed is introduced to all the potential trays. Mariana coupled the MINLP and GDP models with an NLP thermodynamic initialization model that assumes that all the potential trays are present at the final solution. For the MINLP model, a reduction of candidate trays was performed to

decrease the number of trays. From several ternary mixtures that she considered the most effective MINLP model proved to be case (c) (variable feed and reboil). For the GDP the fixed feed proved to be the best. For the MINLP case convergence was only achieved with the initialization procedure. For the GDP case it helped, but it was less critical. In all cases the MINLP models took about one order of magnitude longer time than the GDP models. On the other hand the reduction scheme of the MINLP model produced lower cost solutions than with the GDP models.

Mariana has been studying the extension of her work to the synthesis of superstructures for complex column configurations (e.g. Petlyuk, side rectifiers, side strippers). The superstructure used relies on column sections. Not surprisingly the direct solution for finding the optimal configuration and number of trays is computationally difficult and expensive. The MINLP model proved to be impossible to solve, even with the special initialization procedure. The GDP was better but was also difficult. This motivated a decomposition method to avoid the simultaneous selection of structure and number of trays. The basic idea relies on using the GDP model in which the NLP initialization is first solved with the maximum number of trays for all sections. This is then used to derive an MILP master problem (based on convex hull) for selecting the sections in the superstructure, and followed by another MILP for selecting the number of trays in the selected sections. The reduced NLP subproblem is then solved to obtain an upper bound to the cost. An integer cut is added and the corresponding MILPs are updated. Mariana has applied this scheme to an ideal ternary mixture (n-pentane, n-hexane, n-heptane) that required a total of 6.15 mins, with about 65% of the time being spent in the NLP subproblems.

Dirk Brusis

In the rigorous optimization of distillation processes in GAMS, the description of the thermodynamics is a difficult matter as it greatly influences the performance of the NLP/MINLP optimization in terms of robustness. For instance the calculation of the activity coefficients by WILSON or NRTL models includes several highly non-linear equations to the model, which make it harder to solve. Therefore Dirk explored the possibility of using external functions in GAMS to exclude the thermodynamic equations from the main model. In this way the thermodynamic model for the column is calculated using an external module which can be written in C, Delphi, Fortran or Java and then only the results of the required variables like enthalpies and activity coefficients are passed to GAMS. Dirk solved a ternary mixture first with Wilson. The use of the external functions reduced the number of equations by 40% and the iterations of CONOPT dropped from 783 down to only 32. When using the NRTL model the number of equations was reduced by 60% and the iterations from 1980 to 42! It is interesting to note that the times were not greatly reduced because of the overhead caused by the external functions. The important point, however, is that the robustness is greatly increased, which in fact was verified by changing the starting points.

Jennifer Jackson: Reactive Distillation

This project is currently on hold. Jennifer assumed that in a reactive distillation column one or several feeds of reactants are given, as well as the stoichiometry and kinetics of the reaction that is assumed to occur in the liquid phase. The major decisions are selecting number of trays, the trays where reaction takes place, and the number and location of feed trays. All trays in the column are treated as conditional, except the condenser and reboiler. Both kinetic reaction and phase equilibrium may take place; or else no mass exchange takes place in the conditional trays. The possibility of multiple feed trays is also considered. Jennifer developed a nonlinear disjunctive programming model, which she solved with a variation of the logic-based outer-approximation method of Metin Turkay. Jennifer solved two problems. One was the methatesis reaction in which 2-pentene reacts to give 2-butene and 3-hexene using 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 pentane 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.

Jose Caballero
Jose has addressed the issue of systematically generating all the configurations for thermally coupled distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. Agrawal (2000) has addressed this problem and proposed a procedure to draw by "hand" the thermodynamically equivalent structures. Jose developed a set of logic propositions that can be expressed as constraints in an GDP model to define the search space for these thermally integrated columns. Jose also derived equations to calculate the number of thermodynamically equivalent configurations for a given sequence of tasks. Jose has applied the logic constraints to simplified MILP problems involving mixtures of 4 and 5 components. Jose has also completed the manuscript describing this work, which is enclosed.

Supply Chain Optimization with Process Models and Retrofit Design in Process Networks

Students: Jennifer Jackson [Ph.D., started Jan 99]
New Development: Tempora l vs. spatial decomposition for Multisite-Multiperiod Planning model

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

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

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

As described in the last newsletter, Jennifer has recently started to extend the above model to a supply chain optimization problem involving multiple sites of production and multiple markets in which the transportation of products is considered. The major difficulty becomes the large size of the problem, which makes it very difficult and expensive to directly apply NLP algorithms for the solution. In her initial attempt Jennifer explored the use of Lagrangian relaxation, in which the material flows between plants and markets are dualized, which in turn allows the suboptimization of each system for fixed multipliers to produce upper bounds for the profit. These multipliers are updated with a common subgradient

optimization procedure. While this decomposition scheme seemed to provide encouraging results, it did not prove as effective as we had hoped for. For this reason Jennifer has developed a new decomposition approach that is based on the idea of performing a temporal rather than a spatial decomposition. In particular, what she has done is to dualize the inventory constraints, which decouples the multisite problem into independent time periods.

The results that Jennifer obtained for a problem with 3 production sites, 3 markets and 30 products were very encouraging. Each site's production is modeled as a nonlinear function of capacity, raw material availability, physical properties, operating conditions and blending. There are also constraints to optimize the inventory levels for each product, the distribution of each product to the markets, and the production with respect to the demand forecast. The multiperiod NLP model formulated for a time horizon of 12 months consists of 19,945 continuous variables and 17,098 constraints. The full space solution was obtained in 7075 CPU seconds on a Pentium III 500MHz computer. By applying the spatial decomposition method using Lagrangean decomposition, the solution time was reduced to 897 CPU second. When the temporal decomposition method was applied, the solution time was further reduced to 258 CPU seconds. Jennifer is in the process of writing up a paper on this work.

Supply Chain Optimization of Refineries

Visitor: **Jehoon Song (January-July 2002)**
New development: *Solution algorithm based on rolling horizon with aggregation*

Jehoon's project in Korea deals with multiobjective optimization of supply chain problems. During his visit to our group he concentrated on two problems. The first was to extend the scope of the supply chain for refineries. In the initial version it consisted of supply through vessels, storage tanks, blending, and crude-oil distillation units (CDUs). Jehoon added storage of products, transportation to distribution centers, and finally to retailers. While conceptually this was not a difficult task, it did lead to a considerably larger multiperiod MILP model. Furthermore, by increasing the cycle time from supply to retail this also meant that one had to consider longer horizon times. In the initial version of the model typically only one or two weeks were used. With the new version one had to consider at least one month.

Since increasing both the size of the supply chain and the length of the horizon time led to a much larger MILP, Jehoon found out not surprisingly that MILPs were no longer solvable in reasonable time. As an example he considered a supply chain with 4 storage tanks, 2 blending tanks, 2 CDUs, 3 product tanks, 2 distribution centers, and 4 retailers over a 30 day horizon. The corresponding MILP, which involved 780 0-1 variables, 3021 continuous variables, and 5181 constraints, could not be solved with CPLEX after many hours. This motivated a decomposition strategy, which is as follows. We partition the total horizon into an initial subhorizon with the same time resolution, and the remaining part is aggregated as one period. We then assume that a suset of the initial subhorizon is optimal, and eliminate it from consideration. We next shift the start of the reaming horizon, and repeat this procedure, and stop until the entire horizon is covered. Using this procedure Jehoon could solve the problem for 15-day subhorizons and subsets of 5 and 3 days. The case of 5 days required 4 subproblems that were solved in only 92 secs. The case of 3 days required 238 secs. As one might expect the objective in the latter was better (16,618 vs. 16,022 of profit). Note that in both cases the MILPs over each subhorizon are identical in size. They involved 416 0-1 variables, 1651 continuous variables and 2803 constraints. Finally, it is interesting to note that if one were to take the simple minded approach of simply solving the 30 day problem into a sequence of two 15 day problems the profit reduces to 15,527, which is significantly lower. The computer time, however, was only 56 secs. Jehoon is in the process of writing the paper and completing some final results.

Optimal Design and Planning of Oilfield Infrastructures under Uncertainty (PENDING)

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

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

The specific problem that Vikas has considered is an offshore gas-producing site with a number of reserves of gas, or fields. The size (total recoverable gas from a reserve) and the deliverability (maximum rate of recovery for a reserve) of some of these fields are known with certainty, while those for the rest are uncertain. Given this information, the problem consists in making investment decisions regarding what fields should be exploited and what infrastructure needs to be set up for this purpose. Operational decisions relate to determining the production rates of the fields over time. Vikas' first approach was to consider a two-stage programming strategy in which the selection of well platform and their capacities are considered as stage-1 variables, while the production levels and flows are considered in a second stage. Discrete distribution functions for the sizes of the fields (total recoverable gas) and their quality (maximum rate of recovery). The two-stage strategy can be transformed into a multiperiod optimization problem. The difficulty however, is that the number of scenarios that must be considered for each time period can be very high, leading to a very large scale MINLP problem. As an example a problem with 10 fields involves over one million scenarios. What Vikas then explored is a decomposition scheme that exploits the fact that each well platform has only “major” operating modes corresponding to the discrete realizations corresponding to the well associated with that platform. He applied these ideas to the gas oilfield problem by Sarette. The proposed method by Vikas relies on a Lagrangian decomposition scheme for aggregating the multipliers connecting the production and well platforms, so that the net result is that each well platform must be optimized only for its “major” operating modes, which drastically reduces dimensionality of the multiperiod problem. Vikas applied this scheme to a problem involving 5 fields (2 uncertain), which gives rise to 16 scenarios since there are two discrete probabilities for each parameter (size, quality in each field). Using a full space method (about 10,000 constraints) required more than twice the time (474 sec vs 196 secs). For the case of 3 discrete probabilities (81 scenarios), the proposed method was more than four times faster (3,500 sec vs 15,500 sec). Vikas also showed that the predicted well platform capacities are significantly different when compared with the ones predicted by the deterministic model. The limitation of this method is that the subproblem that remains with the dimensionality of the total number of scenarios, is the optimization of the production platform. More importantly, Vikas also discovered that a subtle point when extending the formulation to a multistage stochastic optimization strategy.

Vikas developed a multistage stochastic programming model for the investment and operational planning of these infrastructures under uncertainty. The reason for going beyond the two-stage programming strategy is the fact that the design decision can take place over any of the multiple time periods (i.e. in multiple stages). The feature that greatly complicates the problem under this strategy is that, unlike the two-stage stochastic programming approach, the scenario tree for the problem depends upon the investment decisions. Or in other words, the sequence of scenarios is dependent of the timing when design decisions are implemented, which in turn then dictates the particular structure of the multistage optimization that is to be solved. To solve the multistage problem Vikas developed an approximate solution technique where the basic idea is to search in the space of scenario trees to find the one that is optimal. In particular, the procedure starts by optimizing the problem independently for each scenario, which provides an upper bound. Next, at every iteration of the algorithm, a specific scenario tree is generated using the solution of the deterministic expected value problem. The multistage stochastic program for each of these trees is then solved in order to yield a lower bound. Since this multistage problem can become very large, we use a rolling-horizon approach combined with Benders' decomposition in order to avoid the simultaneous solution in the full space. The procedure is continued until the lower and upper bounds lie within a given finite tolerance. The solution algorithm was applied to problem with six fields, three of which are uncertain (i.e. 27 scenarios), yielding a solution guaranteed to be within 1% of optimal. Vikas is currently

investigating ways for efficiently updating the subproblems that arise in Benders decomposition in order to reduce the computational time.

Scheduling of Batch and Continuous Multiproduct Plants

Student: **Christos Maravelias (Ph.D. started January 2000)**
New Development *Initial MILP continuous time model for State-Task Network*

Christos Maravelias has been working on this project after Iiro left our group. One of Iiro's projects was the integration of CP (Constraint Programming) and MILP. Iiro developed a strategy for the short-term multistage batch plant scheduling problem that Jose Pinto studied in his Ph.D. work, and is implemented in the STBS interface. The only difference is that Iiro uses as the objective to minimize the cost of assignments to orders to machines, instead of minimizing tardiness. The idea in Iiro's work was to partition the assignment and sequencing decisions by solving a MILP subproblem for the former, and a CP problem for the latter in the spirit of Vipul Jain's hybrid strategy. Iiro, however, also tried to use an MILP for the sequencing phase, as this has the advantage that the same solver can be used. Iiro proposed several cuts, which we found surprisingly difficult to derive. The numerical results showed that it is generally advantageous to use CP for the sequencing part, although the times for the MILP were by no means excessive. As an example, in one of the largest problem (3 stages, 8 machines, 12 jobs), the MILP (CPLEX) required 2767 secs, and the CP (ILOG) required 712 secs. The hybrid strategy required in contrast only 14 secs.

Regarding Christos he has developed a new continuous-time MILP model for the short term scheduling of multipurpose batch plants. His model relies on the idea of Stat Task Network (STN) and accounts for resource constraints (other than units), variable batch sizes and processing times, and various storage policies (UIS/FIS/NIS/ZW). The time domain is treated through intervals in which the continuous events that define the start times of the operations are matched with the start times of the intrvals. The assumption of no batch splitting, which is used in other recently proposed models, is not needed in Christo's model making it more general than previous works, which may either overconstrain the problem, or else produce infeasible solutions. The idea of decoupling tasks and units is used in the representation of the model. These ideas combined with a novel way of expressing assignment and time matching constraints leads to formulations with fewer binary variables. Moreover, a set of logic cuts is added leading to tighter LP relaxations. As an example of the performance of this MILP model Christos solved the classic Kondili problem for12 time periods. The latter required 128 0-1 variables, 1831 constarints and 739 continuous variables, requiring 6.8 secs with CPLEX. Christos has also explored the integration of Constraint Logic Programming. His preliminary findings are that for the profit maximization there does not seem to major advantages. For the case of makespan minimization, however, the trend is reversed. The results with CLP should be completed for the next newsletter.

Uncertainty in the Scheduling of Batch Processes

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

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

In his initial work, Jayanth developed a branch and bound procedure for flowshops with zero wait policy in which the key ideas are the following. First, for a fixed sequence the analytical expression proposed by Karimi is used to simplify computing the expected completion time. The property that the expected value of a sum is the sum of expected values (assuming independence) is then exploited to reduce to few hundreds the evaluations for the expected completion time. The second important property is that when the

tasks in the flowshop are replaced by the expected process times, the completion times yield a *lower bound* to the expected completion time. Third, Jayanth devised a clever branch and bound enumeration in which he sequentially "explodes" the full probability space on products that have been fixed in the sequence. The products that have not been fixed are replaced by expected values, which guarantees the lower bound properties. In the implementation that Jayanth developed in Java he was able to solve problems with up to 9 products and 3 stages with $7x10^{12}$ scenarios. That particular problem, which cannot even be generated for a conventional multiperiod equivalent, required 1600 secs for solving the problem to optimality. Jayanth also extended the method for flowshops with UIS policy and for continuous distribution functions using discretization schemes that rely on the fact that for univariate functions exact discrete approximations are possible for higher moments by the appropriate selection of discrete points that correspond to roots of polynomials for Gaussian integration. Jayanth also addressed the problem of parallel units with uncertain processing times, in which he has been able to exploit similar lower bounding properties. In this case the evaluation of the expected completion time for a fixed schedule can be performed quite effectively. However, the optimization with branch and bound is much harder. Therefore, Jayanth developed a reactive tabu search algorithm to optimize the schedule. Using this approach, he obtained generally good results.

Motivated by the need to develop computationally efficient methods for optimizing schedules with uncertain tasks, Jayanth has developed a non-probabilistic approach that relies on the use of fuzzy sets. In terms of completion times, this is almost equivalent to interval arithmetic where the major result that one can obtain are lower and upper bounds for the completion time for a fixed schedule. Using triangular fuzzy numbers, the equivalent to the expected completion time reduces to the average completion time integrated over all parametric intervals that are centered to the center point, and with deviations proportional to the bounds of the completion time. In order to better understand the relationship of this approach with probabilistic methods, Jayanth developed general guidelines and a specific example, which shows the following. The probabilistic approach requires multiple integrals, while the new approach only involves single dimensional integrals. To extend this approach to optimization one can formulate a corresponding MILP model, which Jayanth did for flowshop plants (single units per stage and parallel units), and for the new product development problem. In the case of flowshops with 12 products and 4 stages (48 uncertain times) the MILP took on average 800 secs. The probabilistic version of this problem is too large and cannot be generated, much less solved. As another comparison with the probabilistic approach in a problem with 8 products and 4 stages, Jayanth's procedure required about 28 sec while the probabilistic approach required 4 hours! Jayanth also developed a reactive tabu search procedure for solving much larger problems. This has allowed him to solve a problem with up to 20 products and 4 stages, and sequence dependent changeover times in 5,000 secs. Solving the corresponding MILP model, after 50,000 secs the problem had not been solved to optimality, and the best completion time found was 295.38, which in fact was slightly lower than the one of the tabu search (303.005). Jayanth has also solved new product development problem with 65 tests, which is a sanitized version of a problem supplied by DowAgro Sciences. The resulting MILP involved 4061 binaries, 8794 continuous variables and 267,912 constraints, and was solved in about 45 minutes with CPLEX.

Jaynath has recently considered the problem of optimizing the short-term scheduling of a multi-product batch plant, while taking into account the uncertainties in the demands for the products. Given are N products that can be manufactured in a batch plant in L modes (characterized by a specific batch size and product-dependent processing time). The demands for these products are described by discrete probability distributions; and these demands are to be satisfied at the end of the scheduling horizon. The costs involved are those for (i) holding inventory over the horizon, (ii) excess inventory at the end of the horizon, (iii) lost demand (due to inadequate production); while the revenues are from selling the products. The problem then is to obtain a schedule that maximizes the expected profit, where the schedule consists of deciding the allocation of the equipment to the appropriate mode of production of a product over the time horizon. Unlike previous work, Jayanth has assumed that some of the demand can actually be unsatisfied, due to limited production capacity. Thus, the problem also consists in choosing the optimal amounts to be produced for each product. Jayanth first developed a deterministic optimization model for maximizing profit as a discrete-time Mixed Integer Linear Programming (MILP) model. To generate robust schedules that account for the uncertainties, the deterministic MILP model was generalized to obtain another MILP formulation, which yields a schedule that is implementable for all scenarios, and has a higher expected profit compared to the deterministic model. Jayanth showed that it is possible to improve on the robust

scheduling approach, by formulating a multi-stage stochastic MILP, where certain decisions are made irrespective of the realization of the uncertain parameters, and some decisions are taken upon realization of the uncertainty. The difficulty with this approach is that the resulting formulation is a large-scale MILP, that is expensive to solve. Jayanth has developed strategies based on solving several successive smaller-scale stochastic MILPs. Examples include single unit processing plants and large State-Task Networks. Among the larger problems solved is an 8-task, 6-unit, 4-product STNs with three possible processing modes for each task over a 18-unit time horizon. The deterministic model for this problem had 456 binaries, and 4000 constraints. The multistage stochastic formulation for this problem had 1104 binaries and almost 23000 equations and could not be solved to even within 10% of optimality in 10 CPU hours. With the strategy of successively solving several smaller stochastic MILPs to approximate the multistage stochastic MILP, Jayanth obtained solutions that improve the expected profit by 18% over solving the deterministic model once, and 6.5% over solving successive deterministic models, in very reasonable CPU time (~10-20 minutes).

Integration of Product Testing and Planning of Batch Manufacturing Facilities

Student: **Christos Maravelias (Ph.D. started January 2000)**
New Developments: *New method using logic implied precedences and decomposition*

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

Based on the continuous time model by Craig Schmidt for scheduling for new product development and its extension by Vipul Jain for resource constraints, and the discrete time linear model for flexible process networks by Norton, Christos was able to integrate both models through a novel MILP model. Furthermore, Christos found a tighter representation of the resource constraints compared to Vipul's work. The proposed model is augmented with scenarios that may arise depending on the outcome of the tests for the products. In order to effectively solve the resulting MILP model, Christos has developed a Lagrangean decomposition scheme similar to Sarette's. In Christos' case the constraints that tie the testing and the manufacturing planning problem are relaxed by dualizing these constraints. The idea then consists of iterating between the dualized problem, which can be decomposed and provides an upper bound to the profit, and a feasible MILP problem that provides a lower bound. Although the gap cannot be guaranteed to be closed, computational experience has been encouraging. One of the examples considered by Christos involves a plant with 4 stages that manufactures 4 products. Two new products are considered in the pipeline, each requiring a total of 10 tests with some precedence constraints. This then also leads to four scenarios in the model. The MILP model involves 718 binary variables, 11,216 continuous variables and 11,173 constraints. With CPLEX it took 57 secs to solve this problem; with Lagrangean relaxation only 37 secs. In a larger example, the reduction was from 830 secs to 252 secs.

Since the major bottleneck in the above procedure is the part of the resource constrained MILP scheduling problem, Christos has revisited that problem, which Vipul Jain had addressed. Christos initially explored a number of alternative solution methods. At the end the most successful approach is one that combines logic cuts with a decomposition procedure. Christos examined the use of both cycle breaking cuts, and cuts for implied precedences. The former cuts are simply to exclude formation of cycles of arbitrary length (2 to n). Christos found that adding these cuts would greatly improve the LP relaxation. To avoid adding all of them

up front, one can add only the ones that are violated in the root node. This means for example in a problem with 2 products (60 and 30 tests respectively) instead of having to add about 90,000 constraints up front, it is sufficient to add about 10,000 that become violated. In both cases the LP relaxation was reduced from 6,176 to 5,698. The second type of cuts are based on implied precedences that can be derived from either fixed precedences, or precedences that arise in the selection of sequences. As an example, if A is followed by B, and B followed by C, then A followed by C is an implied precedence. Christos also applied these cuts in explicit form or as violated cuts in the root node. The former case required adding 239,000 constraints, while the latter required 18,000. Both, however, produced the same reduction of the LP relaxation (6,176 to 5,001) Although the implied precedences greatly improve the LP relaxation, larger problems are still expensive to solve. This motivated the idea of decomposing the problems by products. Those precedences that are activated (i.e. corresponding binaries take value of one) are fixed in the joint problem for all the products. This solution to the overall MILP provides a heuristic, which however, can be shown to have a tight bound. As an example, Christos considered a problem with 4 products with 60, 30, 40, 20 tests, respectively. The full space MILP has 14,000 0-1 variables, 3,300 continuous variables and 26,000 constraints. CPLEX required 6,900 secs to solve the problem with a 5% optimality gap, while the proposed method required 520 secs, finding a solution within 0.5% of the optimum. Christos has written the paper describing this work which is enclosed with this newsletter.

Optimal Multiperiod Planning for Catalyst Replacement (DONE)

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

This project was completed in February by Martin Houze, who has returned to France. The project was a joint collaboration with TOTALFINAELF through Nikola Juhasz. The problem that Martin addressed is as follows. Given is a continuous polymer plant that produces a product with seasonal demands. The process involves a reactor that undergoes catalyst deactivation. Replacing the catalyst is a rather involved operation that requires significant amount of time, as well as careful coordination with the inventory management. Optimization variables in the process include the reactor temperature and the recycle rate, which to some extent can be manipulated to compensate for the deactivation. Given a long term horizon (few years), the problem consists in determining the timing for the replacement of the catalyst, as well as the optimal operating conditions and inventories on a monthly basis.

Due to the complexity of the process, Martin developed a semi-empirical model that provides reasonable fit with the plant data. He used that model as a basis to develop a multiperiod MINLP model for deciding the optimal catalysts replacement, and operating conditions. The model was applied to problems between 2 and 4 years. Despite the presence of nonconvexities, Martin found that DICOPT has almost always found what appears to be the global optimum. Martin implemented the model in a GAMS interface that greatly facilitates the use of the model. This allowed Martin to perform extensive sensitivity analysis. He found that profit is most sensitive to the marginal cost and to the addition of one of the reactants. We enclose a paper that describes the work on this project.

Software for MINLP Optimization in Design and Scheduling

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

Gabriela has completed the web framework for accessing various interfaces through the web. The URL address is: http://newton.cheme.cmu.edu/interfaces
The interfaces that Gabriela has implemented include BATCHSPC, BATCHMPC, CYCLE, DECAY, MULTISTAGE, NETCHAIN, SYNHEAT, and WATER (see brief description below). The web access will make it easier to access these interfaces. Hopefully this will also promote greater use by the members of the CAPD. The idea in the framework developed by Gabriela is that the interfaces all have a "common look" as the current PC interfaces. This project was inspired by the joint collaboration with Dow in which

the final implementation was performed on a web-intranet system. Regarding our collaboration with Zdravko Kravanja, he has continued developing the new code MIPSYN that is PC-based and that makes direct use of the recent developments in disjunctive programming for flowsheet synthesis.

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

Synthesis:

SYNHEAT	MINLP synthesis heat exchanger networks *(Yee)* Also includes transshipment model for targeting *(Papoulias)*
STEAM	MINLP Model for the synthesis of combined cycles for utility plants (Bruno) Model includes correlations for steam, efficiencies and cost data
GLOBESEP	Global NLP optimization for synthesis of separation networks and single feed/mixed products *(Quesada)*
WATER	Global NLP Model for synthesis of wastewater treatment configuration *(Galan)*
EXTRACTOR	Disjunctive MINLP for synthesis of liquid-liquid extraction systems *(Reyes)*

Batch design:

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

Scheduling:

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

Planning:

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

Steinar Hauan's Group

Feasibility and Economics of Reactive Separation Systems

Student: Warren Hoffmaster (Ph.D., started Jan 2000)

BACKGROUND

Over the last decade, the idea of combining reaction and separation has shown a significant industrial potential. As of today, most major chemical companies are considering or implementing processes, such as

reactive distillation columns and membrane reactors along with more well known variants like absorption columns with chemical reaction, multiphase reactors and reactive heat exchangers.

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

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

1) What is the product composition region -- i.e. all product reachable for a given feed – for systems combining reaction and separation?

2) Given a set of feasible processes involving both sequential and simultaneous reaction and separation; where is the economic optimum as a function of system specification and process operation?

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

PROGRESS

Warren is currently validating his techniques for finding reachable compositions against a series of industrial examples and uses these to identify structurally different feasible column designs. By scaling the reactive holdup in each stage by the difference of flowrates entering and leaving the cascade sections, the same equations are now valid for kinetically controlled reactions as well as those with specified turnover or conversion profiles. The examples in question include the "standard" acetates and ethers as well as acetic acid, olefin metathesis and a set of schematic cases with ideal VLE behavior.

Agent Systems in Engineering Design and Optimization

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

BACKGROUND

Co-advised by Art Westerberg, John is studying how to pose and solve very large design and operation problems where:
- the models are complex, highly nonlinear and definitely non-convex
- many of the calculations fail routinely
- the problem has many local optimum
- the solution space of discrete alternatives is enormous

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

John is studying the use of agent-based systems. In these systems many agents attack different or even the same parts of the problem. There are also agents that remove bad solutions. All these agents share total and partial solutions as they progress. This sharing is very low bandwidth relative to the information

developed by any agent internally. Experience shows there is considerable synergy among these agents, often reducing the time to find solutions by surprising amounts. For example, an agent may discover another agent has produced a particularly good new point from which it thinks it can make rapid progress. Or it may find a solution that gives it a much improved bound over any it has found by itself. These systems are like creating an army of ants to attack the problem, in the hopes that one of them will reach a desired solution. Parallelism comes by having the agents operate more or less autonomously and in parallel on several computers. But if computing is fast and cheap - why not?

Our strategy has three algorithmic levels:

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

2. All solution agents are divided into two parts: The preprocessing -- or ‘scouting’ -- step analyze the current state of the problem and estimates a probability of improvement. This is fed back to the resource control agent which may or may not decide to allow the actual 'work' part of the agent to be run. A key point is that not all agents are expected to yield actual solutions; it is perfectly acceptable to use heuristic or statistical rules to deduce, suggest or guess where good solutions may -- or may not -- be found.

3. The meta-agents analyze the performance of the pool of solution agent. This is fed back to the resource control loop to help divide the problem into solution 'phases' and to minimize the waste of resources on agents not suitable for the problem at hand.

PROGRESS

The progress report for John's work is found in Art's section of the newsletter.

Microscale Process Design

Students: Anton Pfeiffer (Ph.D., started Jan 2002) and Michael Bartovsky (Ph.D., started Jan 2002)

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

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

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

Applications are emerging in the areas of sensor systems, microscale chemical synthesis, high throughput screening, environmental monitoring and medical sciences. The goal of this research is to adapt and expand current algorithms for process design into this new domain. At present, two directions are being actively

pursued: (1) microscale fluid flow and chemical reactions, and (2) gravimetric sensing of biological molecules

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

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

PROGRESS

These projects are just getting off the ground with new Ph.D. students officially joining the group in January of 2002.

Anton is working toward a MINLP design model for design of an on-chip separation channel network. From a set of pre-defined channel parts, the MILP topology model selects the optimal component layout. The NLP subpart relates separation resolution and dispersion to the physical channel dimensions and applied electric field. The first step of this work is to capture how analyte bands travel and separate in turns and straight channels as a function of physiochemical properties. While a finite element solution of the convective diffusion equation is possible, it is is very slow (5-30 hrs) to converge as most relevant designs will exist in a transition regime where neither diffusion nor convection dominates the flow patterns. Consequently, PDE solutions are unsuitable as a practical design tool. In the literature, there has been several attempts at approximating the behavior of electrophoretic separation in microchannels. The key factor to take into account are: (a) dispersion of analyte bands in any channel with electrophoresis and -osmosis, (b) the skew angle of a Gaussian band going through a turn, (c) the effect of local (Joule) heating, (d) the non-uniformity of electric fields around a sharp turn, (e) the impact
of buffer and surface properties.

Anton has developed a tool (CHANNELSIM) in Matlab based on component models for turns and straight channel sections. The major contribution so far is how to treat a sequence of turns with interconnecting straights: Asymmetric diffusion in a skewed analyte band entering a straight channel section will cause additional dispersion ("band broadening", up to 40x) compared to the same straight channel immediately following a sample injector. However, these effects may be partially offset by complementary turns wherein skew is "undone" by a sequence of symmetric turns. Verification against finite element simulations show agreement to within 5% for relevant regimes. The models are currently being reformulated to ensure convexity and reasonable limiting behavior in preparation for a mixed integer optimization framework. Collaborators in this project are working to generate algebraic models capturing the detailed effects of points b+d (ECE) and c (MechE).

Mike has made progress two areas: Mathematical modeling of vibrating strings (1D) and membranes (2D) with arbitrary, non-uniform massload. Using the finite element programming package FEMLAB, we can assess the steady state (eigenfrequencies) and dynamical (power spectrum) response of a particular setup.

Preliminary sensitivity calculations show order of magnitude improvements over current techniques based on Quartz Crystal Microbalance (QCM, 6 orders of magnitude) and microscale vibrating cantilevers (2 orders of magnitude). Binding chemistry for are being explored for two protein systems on a separate QCM setup: One reversible and one non-reversible.

In addition, ECE collaborators are working to integrate piezoresistors into the polymer membrane. This would enable integrated actuation and detection and avoid possible contact between the liquid solution and on-chip electronics.

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 developed methodologies 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 proposed to synthesize scenarios. He anticipated where future technology might challenge a process. He explored the use of a so-called "free step" (originally proposed by Bill Johns and his student Romero in the 1977 and 1979). If one can have any step in the process for free, then by how much would the process and its economics change? If a step allows for significant improvement, then it becomes a candidate for assessing the possibility someone might figure out how to do it. Together this information will aid one to assess the possibility such a technological breakthrough could threaten the current design.

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

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

He then demonstrated that he can model events (using ideas that Vicente Rico-Ramirez developed early in his Ph.D. project) non-procedurally. He also demonstrated that he can model queues (e.g., an order can be added to a queue to be processed later), time delays, and so forth, in a non-procedural modeling system (yes, ASCEND). The conjecture is that this approach to developing these models will be very easy for a typical modeler, a conjecture we have yet to prove. It may be hard for a person steeped in the traditions of procedural modeling at first, however, as it will represent a very different way to think. The idea is that one

simply says what has to be true and not the order in which things will happen. The truth can include events happening when something starts to boil, for example, and for the system to alter its modeling equations for times that follow when that happens. You are probably thinking about this procedurally while it is being described here. The trick is to think clearly and easily about it non-procedurally. When (not if) that becomes possible, then we can model both physical artifact and its operation in the same language. The solvers will not care which is which.

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

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

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

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

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

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

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

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

into the problem

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

$$g(z) \leq 0$$

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

Lifei formulated and solved an example problem of this type. He showed the very significant impact of trading off economic benefit with risk.

Recent progress: Lifei has been at Exxon/Mobil since July 1 and will be there until the end of August. While there he is working on closely related stochastic problems.

Before he left, Lifei continued his effort to solve much larger multiobjective stochastic optimization problems. He has proposed to use a parameterized feedback control policy to make decisions. For example, the form for the control law could be to manufacture another batch if inventory falls below a value that is an adjustable parameter to the policy. His goal is to find control policies that are Pareto optimal for his stated objectives over a large number of randomly generated "controlled" scenarios.

To generate the randomly generated scenarios, he first creates one list of random numbers for each scenario he will be considering. These lists remain fixed through the solving process, thus allowing for completely reproducible yet random results. A scenario is to simulate the process. Whenever a random input is needed (e.g., the monthly demand for a product or the sales price), he uses the next number on the random number list associated with it to compute that input. Whenever a design or control decision is needed, he uses the feedback controller associated with that decision along with the current parameters that establish its current behavior. After running all scenarios and evaluating suitably averaged values for the different performance measures, an optimizer adjusts the parameters to seek Pareto points. The conjecture is that he can discover the form for the controller that will allow him to find policies that will be near to the best he could do if solving the very much larger more complete problem formulation.

Agent-Based Large Scale Optimization
Ph.D. student: John Siirola (started August, 2000) (co-directed by Steinar Hauan)

Background: John is looking at how to pose and solve very large design and operation problems where

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

His approach assumes that computing capabilities will increase many fold this next decade. This work continues that started by Ken Tyner on the synthesis of flexible separation processes.

John is studying the use of agent-based systems. In these systems many agents attack different or even the same parts of the problem. There are also agents that remove bad solutions. All these agents share total and partial solutions as they progress. This sharing is very low bandwidth relative to the information developed by any agent internally. Experience shows there is considerable synergy among these agents, often reducing the time to find solutions by surprising amounts. For example, an agent may discover another agent has produced a particularly good new point from which it thinks it can make rapid progress.

Or it may find a solution that gives it a much improved bound over any it has found by itself. These systems are like creating an army of ants to attack the problem, in the hopes that one of them will reach a desired solution. Parallelism comes by having the agents operate more or less autonomously and in parallel on several computers. But if computing is fast and cheap – why not?

John set up an example problem on which to demonstrate the effect of agents helping each other to find solutions. The problem has an objective function comprising the sum of a number of sinusoidal functions with differing frequencies and amplitudes plus a quadratic term. It has many, many local optima. For example for five degrees of freedom, it has $5x10^8$ local optima, with five of them being the global optimum. John created several types of agents. For optimization, he created a gradient-based hill climber implemented in GAMS, a simulated annealer and a genetic algorithm – both in PERL. He also created a "look for places where there is a paucity of points" algorithm. Finally he created an agent to eliminate points that are in regions where no good points have ever been found. He can activate many copies of each of these algorithms, each with different parameterizations so they will behave differently.

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

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

Recent Progress: John has recreated, debugged and tested all his single objective function agents to operate in a new software environment that will make creating agent-based systems much less tedious. He is now working on agents to find Pareto surfaces for multiobjective problems. He continues to use artificial problems having enormous numbers of local optima for the various objectives, which makes the problem extremely interesting and complex. The goal again is to discover how much of an impact agent cooperation has on the effectiveness of the algorithms he includes in his agent-based system.

Visiting Researchers

Gabriela (Gaby) Mannarino, a post doc from Santa Fe, Argentina, continues her work on improving our n-dim modeling environment. She is adding functionalities that allow a user to create multiple views of the information. The view description is largely through the configuration of n-dim models representing the views and by adding operations that can operate on those models. She is also examining how to manage and create new operations, again using n-dim modeling itself to aid in this activity. To particularize her work, she will apply it to create user interfaces to the ASCEND system.

Other Activities

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

a significant issue we meet head on. We grade the teams on their use of our LIRE' document management system to capture, organize and share all information for their projects.

Erik Ydstie's Group

Robust Adaptive Control Using Multiple Models

Students: Jennifer Hill (graduated spring '02)

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

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

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

Distributed Simulation and Control of Process Networks

Students: Vianey Garcia-Osorio

Vianey Garcia-Osorio has tested a new approach for static and dynamic simulation of process methods in a few case studies. The method is based upon the thermodynamic stability and process network theory. The simulation is carried out in parallel over the web and can lead to significant improvements in computational speed and savings in development cost. The current method is implemented in MATLAB/SIMULINK and has been used to simulate single process networks. One unique aspect of Vianey's approach is that the method does not require a central coordinator to stabilize the computation. In this way the simulation is scale-able and very large systems can be simulated without slowing down the execution speed. We have worked with an undergraduate CS minor student to streamline and optimize the code needed to interface a large number of computers over the Carnegie Mellon network. We have engaged an undergraduate student (Nasser Abukdeir) to write protocols for information exchange. These are based on the MPI code and adapted to MATLAB. The methods will be tested for simulation and optimization of large scale chemical process systems.

Modeling and Control Complex Chemical Reactors

Students: Dimitrios Gerorgios
Vianey Garcia-Osorio
Martin Ruzskowski
Marta Duenas-Diez (PhD HiT Norway)

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

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

Vianey Garcia-Osorio models the vapor recovery section of the aluminum process. A significant amount of aluminum vaporizes from the aluminum reactor and this aluminum must be recovered in a vapor recovery column. Vianey models the primary reaction in the column, the gas flows as well as solid transport. She also looks at stability and overall process integration.

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

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

Supply Chain Management

Students: Edgar Perea-Lopez (graduated, spring `02, co-supervised with Prof I. Grossmann)
Ashish Agrawal (co-supervised with Prof I. Grossmann)

In this research we develop new modeling, control and optimization approaches for large scale chemical supply chain systems.

Edgar developed an MILP model for a multi-echelon supply chain involving a manufacturing plant, plant storage, distribution centers and retailers. He coupled the model with an optimization method and developed a model predictive approach for control and optimization of the supply chain. He compared the centralized optimal controller with a decentralized approach and he showed that the optimization based approaches can give significant savings due to better co-ordination of plant schedule, inventory levels and shipping between distribution centers and retailers. He also developed and extensive sensitivity study where he showed that short horizons can lead to very poor policies.

Ashish developed some new results for stabilization and feedback control of the desk-top problem. He has very recently developed MILP methods that he will use to compare heuristic policies with optimal ones. He main contribution to date has been the development of a flexible and comprehensive modeling paradigm for supply chains that allows the application of the formulism of hybrid automata and discrete event modeling. He is currently in the process of developing new computer codes that will allow him to explore the application of new control policies and optimization methods for improved supply chain management.

Thermodynamcis and Process Networks

Students: Luis-Felipe Tavares

The aim of this research is to develop new foundations for control and optimization of large integrated, networks of chemical processes. We use the formalism of irreversible thermodynamics and the passivity theory of nonlinear control as a basis for this theory. However, there are severe limitations that need to be overcome when we extend these methods to problems that include coupled fluid flow, heat and mass transfer.

Felipe has developed new stability results for the flash systems and he is currently studying how he can extend these to distillation by combining his ideas on using the Gibbs-Duhem equation with the algerbraic methods of Chad Farschman and the Lagrangian/Eulerian decomposition of Duncan Coffey. Some progress has been made and is reported in an early paper by Duncan. Much work remains to be done before this theory has the power we expect to need in order to develop control systems in a systematic manner for large scale process systems.

CAPD REPORT SERIES

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B-02-07
S. Kauchali, B. Hausberger, D. Hildebrandt, D. Glasser and L. T. Biegler, "Automating Rector Network Synthesis: Finding a Candidate AR for the Water Gas Shift (WGS) Reaction," submitted for publication (2002).

B-02-08
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B-02-09
Daeho Ko, Ranjani Siriwardane and Lorenz T. Biegler, “Optimization of Pressure Swing Adsorption Process using Zeolite 13X for CO2 Sequestration.”

B-02-10
Maame B. Poku, Lorenz T. Biegler, Jeffery D. Kelly, Ronald Coxhead, Vipin Gopal, “Nonlinear Programming Algorithms for Large Nonlinear Gasoline Blending Problems.”

G-02-05

Balasubramanian,J. and I.E. Grossmann, “Scheduling Optimization under Uncertainty.-.An Alternative Approach,” submitted for publication (2002).

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