CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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GENERAL NEWS

Ignacio Grossmann has stepped down as Head of Chemical Engineering after eight and one half years in that position. Andy Gellman has become the new Head, effective January 1, 2003. Ignacio will take a sabbatical leave in the academic year 2003-04. He will spend the first half in Spain at the Universidad de Cantabria, and the second part in ETH Zürich at the Insitut für Automatik with Manfred Morari. Ignacio was named a Fellow of INFORMS (Institute of Operations Research and Management Science) in the inaugural group of fellows that INFORMS instituted this year in its 50^{th} anniversary.

Art Westerberg will be on leave this next year (translate that to mean, he is "retiring" to do his "thing" at the end of this semester). He will be working with Ben Allan at Sandia Lab to improve the ASCEND modeling environment. His first efforts will be to improve its ability to handle initial value problems and to make software components out of the ASCEND solvers.

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.

Art Westerberg has just been informed that he won the CACHE AWARD for Excellence in Computing in Chemical Engineering Education, ASEE, for 2003.

We welcome the following new students into the CAPD area. *Juan Arrieta* from Iberoamericana University in Mexico City and *Seth Knaebel* from CMU will be working with **Larry Biegler**, *Maria Garcia* from ITERM, Monterey will be working with **Ignacio Grossmann**, Gabriela Garcia, who has been working as a researcher, will be working under Ignacio for her M.S. degree. Ashish Agrawal has been reassigned as Ignacio's Ph.D. student. *Xiang He* from Xian Jiaotong University will be working with **Steinar Hauan**, *Calvin Chan* from Cooper Union will be working with **Gary Powers,** and *Kendell Jillson* from the University of Massachusetts and *Christy White* from the University of Arkansas will be working with **Erik Ydstie**

Jennifer Jackson has completed her Ph.D. degree with Ignacio and will be joining McKinsey & Company in June. Carlos Mendez, a graduate from INTEC in Argentina, and who worked under the supervision of Jaime Cerda for his Ph.D., has joined Ignacio's group as a postdoc to work on joint projects with ABB and BP. Lorena Bergamini, from INGAR, Santa Fe in Argentina, has also joined Ignacio's group for a six month stay. She is working in the area of global optimization.

Sangbum Lee, who worked with Ignacio in his Ph.D. studies and more recently as a postdoc, has joined the research group of Costas Maranas at Penn State to do research in the area of bioinformatics. Veronique Bizet, a student from France sponsored by Atofina Chemicals, has joined Ignacio's group to continue work in the catalyst management problem that was initiated with Martin Houze. Mariana Barttfeld, who spent over one year in Ignacio's group doing research in the area of distillation optimization in collaboration with Pio Aguirre from INGAR has returned to Santa Fe, Argentina, to complete her Ph.D. work. Lorena Bergamini from that group in Santa Fe, will join Ignacio early in January for a one semester stay. Also, Carlos Mendez, who recently completed his Ph.D. under the direction of Jaime Cerda at INTEC in Argentina, will join Ignacio's group as a postdoc to work in a joint project with ABB.

Nicolas Sawaya has successfully passed his Ph.D. qualifying exam and Vikas Goel has also successfully passed his Ph.D. proposal exam.

Tobias Jockenhoevel returned to Germany after completing his stay at CMU on the development of the OptControlCentre. He is currently completing his Ph.D. thesis at the Technical University of Berlin and has joined Siemens AG. Sebastien Gros recently returned to EPFL, Lausanne; he had visited Larry Biegler's group and worked on combining analytic and numerical methods for optimal control. Dr. Soledad Diaz is currently visiting Larry's group as a Fulbright Fellow. She is working on large-scale dynamic optimization of ethylene processes.

PSE 2003

Prof. Bingzhen Chen (Tsinghua University, Beijing, P.R.China) and **Art Westerberg** are co-Chairs of PSE 2003 (http://pse2003.chemeng.tsinghua.edu.cn/), the eighth in the triennial series of international symposia on process systems engineering initiated in 1982. The conference will be held June 22-27, 2003 in Kunming, Yunnan Province, P.R.China. The purpose of PSE meetings is to bring together the worldwide PSE community of researchers and practitioners who are involved in the creation and application of computing based methodologies for planning, design, operation, control, and maintenance of chemical processes. The special focus of pse2003 meeting is on the topic of how these PSE methods and tools can support the high-level business decisions required in the process industries. We hope that many of you will be able to attend. We expect it to be a meeting that helps define a future focus for PSE research.

FOCAPO 2003

Ignacio has co-chaired together with Conor McDonald the FOCAPO (Foundations of Computer Aided Process Operations) 2003 Meeting that took place on January 12-15, 2003, in Coral Springs, Florida. The theme of the meeting was "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. About 140 participants were registered: 45 from industry and 95 from academia. Companies represented included ExxonMobil, Shell, BP, TotalFinaElf, DuPont, Dow, Bayer, Eastman, Mitsubishi, Air Products, Eli Lilly, Procter & Gamble, ABB, AspenTech, i2, SAP, ILOG, Dash Optimization, SmartOps, Accelics, Intelligen, Pavilion, and Slim Technologies. 50% of the participants were international from 25 countries.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* will be offered on April 30-May 6, 2003. In the past we were very pleased with the outcome of this course. Last year 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 Wednesday and Thursday (April 30-May 1), with focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.

b) Optimization - taught on Friday and Saturday (May 2-3), with focus on modeling and algorithms for nonlinear programming and mixed integer programming including disjunctive programming and applications to process optimization.

c) Process Operations - taught on Monday and Tuesday (May 5-6), 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 will be distributed in electronic form. We would appreciate receiving feedback from our member companies of our CAPD website, **http://www.cheme.cmu.edu/research/capd/.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Other websites of interest are Ignacio's http://egon.cheme.cmu.edu, and Larry's http://dynopt.cheme.cmu.edu. Also, the department maintains the website of CEPAC (Chemical Engineering Pan American Collaboration), the organization that has been formed to promote collaboration between the US and Argentina, Brazil and Chile. You can find in **http://cepac.cheme.cmu.edu** a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada and Chile. Mexico's will be added soon.

CAPD REPORT SERIES

Along with 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

Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the reduced Hessian SQP (rSQP) strategy along several directions. A somewhat older 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** and **Vanesa de la Torre**) as well as other fuel cell systems (**Cong Xu**). **Andreas Waechter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, called IPOPT, based on many of these SQP concepts. This has been used to solve problems that incorporate a number of specialized decomposition strategies and for a wide variety of applications with up to 2 million variables. IPOPT is available under an Open Source software license; more information on downloading and distribution is given below. The IPOPT strategy has spawned exciting applications to challenging problems in process engineering. First, **Arvind Raghunathan** is extending the IPOPT algorithm to deal with Mathematical Programs with Equilibrium Constraints (MPECs); these arise frequently in many engineering systems. In addition, **Maame Poku** is applying IPOPT, its extensions to MPECs, and its AMPL interface, to blending problems. Finally, **Roscoe Bartlett,** now at Sandia National Labs, has developed a comprehensive suite of optimization routines called rSQP++. Written in C++ with numerical routines in FORTRAN, this suite was demonstrated on a wide variety of optimization applications. rSQP++ will be available under Open Source software licenses and more information on distribution will be in the next newsletter. In a new project, **Carl Laird** is extending the work of Roscoe by incorporating the IPOPT algorithm as well as large-scale extensions into rSQP++.

In addition, **Yi-dong Lang** has developed a user-friendly version of dynamic optimization methods. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called DynoPC, runs under Windows with a GUI interface. It has been distributed to several CAPD members and can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package has been enhanced further by incorporating the ESO CAPE-OPEN modeling standards currently used in gProms. In a parallel effort, we are working with researchers **Tobias 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** and **Sebastien Gros** are expanding the work on dynamic real-time optimization using OCC for singular control problems, as well as deriving theoretical properties of this approach.. Finally, **Nikhil Arora** has the use of trust region methods for data reconciliation problems, gross error detection and EVM problems. A trust region code, called NTREST is being refined and is planned to be available for future release.

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

In the area of optimization **Nicolas Sawaya** has been developing cutting plane techniques for linear disjunctive programming, and has successfully tested them on the stock cutting problem. **Sangbum Lee**, completed 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 http://www.ceride.gov.ar/logmip/ that can transform disjunctive problems with linear constraints into MILP problems with big-M constraints or convex hull reformulations. **Ashish Agrawal** is investigating for supply chain optimization a novel framework based on a hybrid system model that relies on the use of automata and that can be formulated as a generalized disjunctive program.

In the area of process synthesis **Mariana Barttfeld** has completed work on a new decomposition strategy based on thermodynamic initialization and disjunctive programming for the synthesis of complex column configurations that rely on tray-by-tray models. She has also solved recently a challenging azeotropic distillation problem. **Jose Caballero** in Alicante is developing a hybrid STN/SEN superstructure for synthesizing thermally coupled columns using short-cut models.

In the area of planning and scheduling **Jennifer Jackson,** who has recently graduated, completed the work on a new temporal decomposition of a multisite, multiperiod optimization planning model using Lagrangean decomposition, and compared it to a spatial decomposition. **Vikas Goel** has developed a novel and elegant stochastic optimization model whose scenario tree is dependent of design decisions for the optimization of gasfields with uncertain sizes and productivities. He has also developed a novel solution algorithm that yields order of magnitude reductions in computation. **Jayanth Balasubramanian** has completed the work on short-term batch scheduling problem with uncertain demands. Using as a basis a discrete time STN model, he has developed a novel multistage-stage programming strategy that relies on a shrinking horizon solution strategy that involves solving smaller two-stage programming MILPs. **Christos Maravelias** has completed the development of a new continuous time MILP model for STN batch scheduling, which aside from being general and computationally effective, can be shown to be rigorous compared to previous work. Christos has also developed a novel hybrid MILP/CP strategy for solving these problems with alternative objectives (profit maximization, makespan minimization) achieving reductions of several orders of magnitude in the computation. **Gabriela Garcia** has completed the interface GDP-DISTILL on the web for optimal design of distillation columns, which implements the recent model by Mariana Barttfeld.

Steinar Hauan's Group

In his work on design algorithms for reactive separation processes, **Warren Hoffmaster** has developed a method for combining feasible product composition regions with optimal control to produce tradeoff curves between the minimum number of stages and the minimum amount of reactive holdup. When extended also to include energy usage, this approach allows for a rigorous comparison between design alternatives without explicitly considering cost. The second branch of Warren's work involve characterization of reactive pinch point curves; a necessary element in determining feasible regions above.

John Siirola (co-advised by **Art Westerberg**) has demonstrated his agent system for solving large-scale engineering design problem on a multi-objective synthetic optimization problem. Along with numerous refinements of the individual agents and creating multi-objective performance metrics, John has also demonstrated the effect of dynamic changes in the resource allocation system during the solution process

and is working to ensure our measurements are not affected by hardware limitations in physical network and organization of the shared memory.

Anton Pfeiffer has extended and improved the computational efficiency of his algebraic simulation model for the behavior of microscale electrophoretic separation systems. The simulator has been used to study the performance of chip-based channel systems with variable topology in confined areas. Depending on fabrication techniques, species properties and the available voltage sources and end-of-pipe detection techniques, the system exhibits non-obvious tradeoffs between channel topology and separation feasibility and quality. Present work aims at using rigorous optimization for distributing channel sections to cater for situation where use of the full chip area is suboptimal.

Mike Bartkovsky and **Jane Valentine** continues their work toward creating a MEMS-based biosensor based on shifts in resonance frequency due to chemical bindings. In late February 2003, we received the first batch of approx 700 chips from the CMOS foundry with integrated electronics; the MEMS engineer in ECE is working to prepare them for vibrational testing in air. Mike has used our laser engraver to create a liquid reservoir in acrylic plastic that should clamp directly on the chip when mounted in a standard (DIP) pin-package. Jane is deriving models for vibrational frequency as a function of variable mass loading and also attempts to predict the optimal chemistry test system by predicting frequency shifts as a function of mass loading and projected surface density of target molecules.

In February, **Adesola Amosun** (MSc student in ChemE) joined the group. He will work on Artificial Intelligence techniques for identifying and quantifying features and patterns in the datasets generated by **John Siirola's** agent system.

New measurements of our cluster capacity revealed that the new CPUs installed in September were far more efficient than we thought; theoretical peak capacity for the cluster is estimated to 275 gflops/s.

Art Westerberg's Group

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 has postulated strategies to reformulate these problems so they can be solved and continues the writing of a position paper as well as the code to test his proposals for example problems.

John Siirola, working with **Steinar Hauan** and **Art Westerberg**, has developed agents to discover the trade-off surface (Pareto front) for multiobjective problems. Thorough testing demonstrates a significant improvement in performance for the same consumption of computer resources when diverse agents collaborate. He has also demonstrated a significant impact of dynamically altering the mix of agents as the problem progresses. His next efforts are to handle constraints and integer variables.

A postdoc with **Art Westerberg**, **Gabriela Mannarino**, from Santa Fe, Argentina, continues the implementation of a new personal version of n-dim. Multi-person collaboration will occur when each shares his/her personal models through a global version of n-dim.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

rSQP++: A Framework for Large Scale Optimization Strategies

Student: Carl Laird (Ph.D. started Fall, 2001)

In his thesis, Roscoe Bartlett, currently at Sandia National Laboratory in Albuquerque, NM, 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. Moreover, he has extended 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.

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 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.

As part of an ITR project, Carl Laird is currently working on extensions to rSQP++ for PDE-constrained optimization. In particular, he has augmented rSQP++ features to include the filter line search from Andreas Waechter along with a barrier method for NLPs (see description of IPOPT below). Combining this barrier approach with the flexibility of rSQP++ allows us to address much larger optimization problems while taking advantage of particular forms of matrix decomposition (e.g., dense, banded, sparse, iterative) and also exploit advanced computing architectures, particularly parallelism. In the future, this activity will allow us to address multiperiod problems for design under uncertainty as well as large-scale dynamic optimization problems within rSQP++.

Large-Scale Optimization for Partial Differential Equation Models

Students: **Gregory Itle (Ph.D. student started Fall, 1998)**
Cong Xu (M.S. 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.

Previously, 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. More recently, Greg has looked at the optimization of Catalytic Partial Oxidation reactors, modeled in MPSalsa.

Finally, Cong Xu is investigating optimization problems arising in fuel cell applications. Also, he is extended simple DAE models for fuel cells to consider optimal flow patterns and minimization of contamination effects due to membrane crossover. 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)**
Carl Laird (Ph.D. started Fall, 2001)

This project considers an efficient strategy for solving nonlinear programs using interior point (IP) methods, developed by Andreas Waechter, currently at IBM Watson. The resulting approach works either in the full space or can take advantage of the particular 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. 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. The current version of this code can be downloaded from: http://www.coin-or.org.

The IPOPT code is being widely used in Larry's group. Examples include both full space and reduced space versions for dynamic optimization, in OCC and DynoPC, respectively. In addition, the full space approach is used in blending applications and in the solution of MPEC problems. More information in these projects are given below. As mentioned above, Carl Laird is integrating this algorithm to the optimization framework in rSQP++.

Mathematical Programs with Equilibrium Constraints (MPECS)

Students: **Arvind Raghunathan (Ph.D. started Fall, 1999)**
Maame Poku (Ph.D. started Fall, 2000)
Dr. Soledad Diaz (postdoctoral visitor from PLAPIQUI, started March, 2003)

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

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

Arvind Raghunathan has incorporated the MPEC formulation into the IPOPT code along with algorithmic modifications to treat the complementarity constraints more efficiently. This code has been interfaced to the AMPL modeling system and has been tested on a set of library MPEC problems. Our results show that this implementation compares well against competing barrier algorithms such as LOQO.

Arvind tested this approach on a number of process optimization problems with phase equilibrium constraints. These include distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies. Arvind has also dealt with modeling a number of two level optimization problems that arise in engineering applications. In particular, Dr. Soledad Diaz is collaborating with Arvind to extend the MPEC problem to dynamic systems relating to models of cryogenic distillation processes.

Most recently he considered the parameter estimation of a metabolic reaction pathway in *Saccharomyces Cerevisiae*. Here the metabolic model was formulated as a linear program. Its KKT conditions were then embedded within a parameter estimation problem to form an MPEC, which was solved directly by the modification in IPOPT.

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.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Students: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
Seth Knaebel (MS started Fall, 2002)
Researcher: **Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Visitors: **Tobias Jockenhoevel (Technical University of Berlin)**
Sebastien Gros (EPFL)

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. An interesting application of this approach has been adapted to aircraft conflict resolution and is described in a paper listed below. 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.

First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called DynoPC. Written for Windows with a Visual Basic user interface and with heavy integration of graphical, simulation and automatic differentiation tools, this software package incorporates our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from http://coin-or.org Current developments with DynoPC include a collaboration with Prof. Marquardt's group at the Technical University at Aachen (RWTH). Here we have incorporated ESO interfaces, developed by the gProms group that are compliant with recently developed CAPE-Open protocols. This leads to an interface compatible with a number of existing process models and modeling environments. In particular, Yi-dong has recently completed a polymer reactor study that was modeled in gProms and solved with DynoPC. This problem had over 300,000 variables and was solved in about an hour of CPU time.

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 incorporated the IPOPT algorithm within OCC (see http://www.optcontrolcentre.com), a MATLAB-based package for on-line optimization, system identification, off-line steady state and dynamic optimization and process monitoring. In particular, this package incorporates a number of discretization strategies (Gauss and Radau collocation, implicit Euler and BDF formulas) as well as the full algorithmic, graphical and modeling capabilities of MATLAB. With this collaboration we are exploiting the benefits of a MATLAB interface for dynamic optimization. This approach was applied to the dynamic optimization of the Tennessee Eastman challenge problem. Moreover, Sebastien Gros and Shiva Kameswaren are applying OCC to new NLP formulations that yield accurate solutions to singular control problems. 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.

Optimization of Pressure Swing Adsorption Systems

Student: **Ling Jiang (Ph.D. started Fall, 1999)**
Researchers: **Vanesa de la Torre (PLAPIQUI)**
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 sequential approaches are easy to construct and have seen a lot of previous development in other research groups. An important (and time-consuming) aspect to these sequential strategies is obtaining sensitivities from the dynamic model efficiently. Fortunately, recent projects by Barton at MIT, Petzold at UC-Santa Barbara, and researchers at the Max Planck Institute have led to excellent software implementations that calculate sensitivities efficiently from large DAE process models. Also, these sequential approaches take advantage of 'off-the-shelf' solvers and do not require a heavy research investment as with simultaneous methods. As a result, we are embarking on large-scale dynamic optimization projects that combine our large-scale rSQP tools with efficient DAE solvers and sensitivity codes.

To take advantage of these algorithms, we are finishing up on 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 has been spending her summers at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, and automatic differentiation codes, like ADIFOR, to adsorption bed models created from the method of lines. In particular, she concentrated on developing detailed PSA bed models with hyperbolic and parabolic components that require special mass conserving discretization strategies to convert them to DAEs. Termed flux limiters, these discretizations allow the accurate tracking of steep fronts and discontinuities that frequently arise in PSA systems. Ling has successfully simulated and optimized cyclic steady state conditions for two PSA units, using Newton-type and tailored rSQP solvers. From this point she has demonstrated a framework that includes constrained simulation problems and design optimization problems on a number of PSA examples. *Preliminary results of her work show that this optimization strategy can reduced the power requirements for PSA systems by about 15% and the computational cost is an order of magnitude less that with conventional case study approaches* .More recently, she has implemented this approach to run in parallel on our Beowulf cluster; this leads to tremendous speedups in PSA optimization, as the sensitivity equations are trivial to parallelize. Results of this parallelization are described in a paper listed below. 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.

Data Reconciliation for Steady State and Dynamic Processes

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

Nikhil Arora successfully passed his PhD exam and has accepted a position with PraxAir in Tonawanda, NY. For his thesis, he extended data reconciliation and parameter estimation strategies to both steady state and dynamic processes. Initially, he applied statistical tools to determine steady state conditions, classify measurements and observed model variables, detect data outliers and estimate model parameters. In particular, Nikhil investigated more general classes of M-estimators for gross error detection within a simultaneous optimization framework. In particular, Nikhil has applied these approaches to an industrial project on carbothermic processes for silicon metal refining and casting. For these processes, dynamic furnace models are being developed (with Martin Ruszkowski and Prof. Erik Ydstie) and efficient strategies are needed for data reconciliation and parameter estimation for the existing process.

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.

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. Our results with this algorithm, called NTREST (Nonlinear Trust Region Estimation), have shown that these approaches are more reliable than and just as efficient as general-purpose NLP strategies. These are currently being incorporated within a large scale SQP framework as well to take advantage of rapid convergence. This approach is currently being extended to EVM problems as well. Moreover, this algorithm was applied to a challenging parameter estimation problem arising from a polymer reactor model. Applied to a number of cases, Nikhil was able to determine solutions to a variety of poorly conditioned parameter estimation problems.

Finally, Shivakumar Kameswaran recently passed his PhD qualifier 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

Student:	**Nicolas Sawaya [Ph.D., started Jan02]**
Postdoctoral fellow:	**Sangbum Lee [started May 2002, completed December 2002]**
Research collaborator:	**Aldo Vecchietti**
New Developments:	*Cutting plane method and testing in stock-cutting problem* *Completion of superstructure optimization 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). There are two major issues that arise in the continuous relaxation based on the convex hull for linear or nonlinear problems: (a) the corresponding formulations may lead to a problem of large size due to the disaggregation of variables; (b) the corresponding relaxation may produce a lower bound similar or equal to the one obtained from the big-M reformulation of the GDP. One objective in Nick's work is to investigate whether one can theoretically determine whether the convex hull relaxation is strictly tighter than the big-M reformulation. The motivation here is to determine whether there is or not a gain in performing the convex hull reformulation. A second objective is to develop effective solution methods of GDP problems that may exhibit poor relaxations. The test problem that Nick has selected for this purpose is the stock-cutting problem. The idea here is to ultimately develop hybrid methods that rely on cutting planes and constrained programming techniques.

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 Lagrangean 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 Nick 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.

Nick has been examining the solution 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. Nick has formulated this problem with big-M constraints, convex hull reformulation and a cutting plane technique. The latter relies on solving the 0-1 relaxation of the big-M formulation first, followed by a separation problem to generate the most violated cutting plane in the convex hull. This cut is then added to the relaxation big-M model and the sequence of iterations continues until the improvement in the lower bound is below a specified tolerance. At that point a branch and bound search procedure is performed. Using CPLEX 7.5 the solution of a 10 rectangle problem required 437,000 nodes and 252 secs, while the convex hull required 19,000 nodes and 83 secs. Adding two cuts in the root node reduced the number of nodes to 11,300 nodes and the total time to 25 secs

(including separation problem). Adding four cuts reduced the number of nodes to 3,600, although the time increased to 35 secs. This was due to the fact that the euclidean norm was used to solve the separation problem, which led to an NLP. Subsequently the infinity norm was used, with which the timed was greatly reduced since then the separation problem reduces to an LP.

Work is in progress by Nick who is currently examining the possibility of integrating the cutting planes of the GDP with constrained programming.

Sangbum Lee

Sangbum, who is currently a postdoctoral fellow with Costas Maranas at Penn State, completed a special project in collaboration with BP (Jeff Logsdon and Mike Foral) that deals with the superstructure optimization of an olefins plant. Sangbum 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 direct use of equations of state was attempted, but proved to be numerically very difficult to solve. Therefore, the accuracy of the model was improved by empirical modifications of Raoult's law for the hydrogen and methane. Despite limitations in the accuracy, the model proved to be useful in synthesizing designs that led to significant reductions in cost, particularly in the energy use. Also, the multiperiod solution of these problems was addressed. Since the problem can become too large for this case Sangbum developed an approximation strategy. The idea is to solve the problem for each period independently to obtain a lower bound on the cost. The structure of each design is then fixed and equipment sizes and energy cost is optimized for the other periods not considered in that design. Each of these solutions lead to feasible designs and an upper bound to the cost. Integer cuts are derived for the independent design optimizations, and then iterations continue until the difference of bounds is small. Sangbum found that this procedure usually converged in only two iterations.

Aldo Vecchietti: LOGMIP and modeling issues

Aldo and his students at INGAR in Argentina are developing the LOGMIP code, which is as an extension of the GAMS modeling language for posing logic/disjunctive problems. The main features of LOGMIP are several language constructs in order to concisely formulate GDP problems. The syntax that he developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. An interesting related development has also been to show that logic constructs that are commonly used in Constrained Logic Programming (CLP), such as implications for constraints (eg g(x) 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 produced an new version for the implementation of the convex hull relaxation and big-M transformation for linear problems. The main difference with the first version is that it automates the entire solution procedure, and furthermore the language now supports indexed disjunctions. Aldo has implemented LOGMIP in the IDE version of GAMS and tested it with small and medium sized problems that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. Aldo has also automated the logic-based OA algorithm, which is suitable for nonlinear GDP process network problems. An example of part of the input in GAMS that can be accomplished with LOGMIP is shown below:

```
DISJUNCTION D1,D2;

D1 IS
```

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

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

As for the more impressive numerical results with LOGMIP, in one of Jennifer's models, Aldo found that the big-M formulation of her retrofit planning problem takes about 1745 nodes with OSL, while convex formulation through LOGMIP only requires only 9 branch and bound nodes! For more information on LOGMIP see, http://www.ceride.gov.ar/logmip/

Modeling and Optimization of Hybrid Systems for Supply Chain Problems

New developments: *Network representation that includes hybrid automata*

Students: **Ashish Agarwal [Ph.D. , started Jan 00]**

The objective of Ashish's project is to develop a new hybrid systems framework for modeling supply chain networks. This project was originally in collaboration with Erik Ydstie. The basic idea in Ashish's project is to rely on a hybrid dynamic systems representation that combines differential equations to capture the continuous dynamics and automata to capture the discrete dynamics. Each automaton describes the space and dynamics of a single discrete variable. The continuous dynamics is used to represent material flow, while the discrete dynamics is used to model scheduling decisions. The hybrid dynamic representation is then applied to a supply-demand network in order to provide a formal representation of the system, determine the optimal operating conditions, scheduling deliveries, selecting between outsourcing and production, and performing a dynamic allocation of resources. In terms of the optimization of a supply-demand network, the problem can be viewed as finding the trajectory which maximizes profit by enabling multiple transitions during a range of times; the free variables are which state to transition to and when to transition. Two major classes of problems can be considered. Optimization over a finite horizon for which initial conditions are specified, and infinite horizon, for which one can either apply a cyclic policy, or else a model predictive control approach. For both cases Ashish has formulated the optimization problem through a continuous time representation, and where the automaton is represented through disjunctions. Ashish has tested the model formulation on a resource constrained production problem, and on a switched server system (i.e. desktop problem). Numerical results in the latter problem indicated that the optimization model yielded significant improvements in both the finite and infinite time horizon case compared to a heuristic feedback controller.

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: *Decomposition technique for optimizing complex columns with tray-by-tray*
Logic constraints for thermally integrated columns

Students: **Mariana Barttfeld (Ph.D. INGAR), Jennifer Jackson [Ph.D. , started Jan 99]**
Collaborators: **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.

Mariana Barttfeld

Mariana stayed with Ignacio's group for one year in a collaboration with Prof. Pio Aguirre from INGAR in Argentina. She first performed a comprehensive comparison between MINLP and GDP models for optimal design of distillation columns in which several representation of the superstructure based on tray-by-tray models were used. Mariana coupled the MINLP and GDP models with an NLP thermodynamic initialization model that assumes that all the potential trays are present at the final solution. For the MINLP model, a reduction of candidate trays was performed to decrease the number of trays. From several ternary mixtures that she considered the most effective MINLP model proved to be case of variable feed and reboil location. For the GDP the case of fixed reflux, feed and reboiler trays, and all other as conditional trays, proved to be the best. 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 completed most of the work for the synthesis of superstructures for complex column configurations (e.g. Petlyuk, side rectifiers, side strippers), and that uses the tray-by-tray models she studied for individual column design. The superstructure is based on the reversible distillation sequence model by Fonyo (1974) for which Mariana has developed both STN and column superstructure representations, for both zeotropic and azeotropic mixtures. Not surprisingly the direct solution for finding the optimal configuration and number of trays is computationally difficult and expensive. This motivated a decomposition method in which the basic idea is to consider first the selection of column sections, and next the selection of trays for the selected sections. A GDP model was first formulated, which is solved aqs follows. The NLP thermodynamic initialization is first solved with the maximum number of trays for all sections. This is then used to derive an MILP master problem (based on convex hull) for selecting the sections in the superstructure. This model then selects the sections for which another MILP is formulated for selecting the number of trays in the selected sections. The reduced NLP subproblem is then solved to obtain an upper bound to the cost. An integer cut is added and the corresponding MILPs are updated. These are then solved to generate new configurations based on sections, and number of trays. Mariana has applied this scheme to an ideal ternary mixture (n-pentane, n-hexane, n-heptane) that involved a maximum of 15 trays per section. This gave rise to a GDP model involving 96 boolean variables, 3200 constraints and 3300 continuous variables. The total time required was of 465 secs. The solution yielded two columns with thermal integration, which led to the elimination of a condenser. The total cost was $127,000 compared to $153,000 for the direct sequence. Mariana has completed in Argentina an example of an azeotropic mixture (methanol, ethanol, water). in which she used a superstructure with 5 columns. The GDP involved 210 discrete variables and about 10,000 continuous variables and constraints, and was solved in 64 minutes, yielding a two column configuration.

Jennifer Jackson: Reactive Distillation

In this project 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
As described in the last newletter, Jose has been addressing the issue of systematically generating all the configurations for thermally coupled distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. Agrawal (2000) has addressed this problem and proposed a procedure to draw by "hand" the thermodynamically equivalent structures. Jose developed a set of logic propositions that can be expressed as constraints in an GDP model to define the search space for these thermally integrated columns. Jose also derived equations to calculate the number of thermodynamically equivalent configurations for a given sequence of tasks. Jose has applied the logic constraints to simplified MILP problems involving mixtures of 4 and 5 components. Jose is currently developing nonlinear GDP models based on STN superstructures for synthesizing thermally integrated columns using short-cut models.

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

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

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

Jennifer has essentially completed the extension of the above model to a supply chain optimization problem involving multiple sites of production and multiple markets, and 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. Jennifer first developed a spatial Lagrangian relaxation method, 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. This decomposition scheme has not only the limitation that it is not very easy to find feasible solutions for obtaining lower bounds, but can often lead to suboptimal solutions that are not very close to the optimum. For this reason Jennifer developed a new decomposition approach that is based on the idea of performing a temporal rather than a spatial decomposition. The specific idea is to dualize the inventory constraints, which decouples the multisite problem into independent time periods. This has the advantage that the plants and markets are simultaneously optimized for each time period, with which it is also much easier to find feasible solutions for obtaining lower bounds.

Jennifer first applied the spatial and temporal decomposition to a simplified supply chain consisting of 3 plants and 3 plants described by linear plant models. This example clearly showed that for the same number of iterations (40) the temporal decomposition yields a solution very close to the optimum, while the spatial method produces solutions of lower quality. Jennifer also solved a problem with 3 production sites, 3 markets and 30 products. Each site's production was modeled as a nonlinear function of capacity, raw material availability, physical properties, operating conditions and blending. There were 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.

Optimal Design and Planning of Oilfield Infrastructures under Uncertainty

Students: **Vikas Goel (Ph.D. started January 2001)**
New Developments: *Variable scenario tree multistage stochastic optimization of gasfields*

Vikas, who recently successfully passed his Ph.D. proposal, has been continuing the efforts of Sarette in the area of oil and gasfield planning, with the major focus of the work being the handling of uncertainties. He is using as a basis the deterministic models by Sarette that deals with gas fields and in which we do not consider the drilling of wells, but we consider possible interconnections between wells platforms. While Sarette considered complex objective functions that include royalties, taxes and tariffs, Vikas has considered the Net Present Value. Also, given the complexity of the stochastic problem, Vikas has considered a simplified MILP model.

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. 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. 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).

While the two-stage programming strategy described above seemed like a reasonable way of tackling the problem, Vikas for considered the extension to multistage programming which seemed better suited for our problem. But then it is here where Vikas discovered a very subtle point that is rarely covered in stochastic optimization. The specific point is that since the size and deliverability are "endogenous" parameters rather than "exogeneous" (e.g. prices), this means that the scenario trees are actually dependent of when the decisions are made. As an example, if the uncertainty is price, we can have low (L) and high (H), and we have 2 periods, then there are a total of 6 scenarios in the tree: period 1 (H or L), period 2 (HH, HL, LH, LL). On the other hand if the uncertainty is size, then if the platform is installed in period 1, the scenarios are period 1 (H or L), and also period 2, since once the platform is installed the uncertainty is resolved. If on the other hand the platform is installed in period 2 then in period 1 there is only one scenario (i.e. H or L is irrelevant), while in period 2 there are 2 scenarios (H or L). The implication of this observation is that for endogenous variables, the structure of the tree of scenarios is *dependent* of when the decisions are made. Based on this fundamental observation, Vikas formulated the variable scenario tree/multistage optimization problkem as a hybrid MILP/GDP problem, where the disjunctions are used to define the structure of the scenario tree. To solve this difficult problem, Vikas developed an approximate solution technique where the basic idea is to search in the space of scenario trees to find the one that is optimal. The procedure starts by optimizing the problem independently for each scenario, which provides an upper bound to the NPV. Next, at every iteration of the algorithm, a specific scenario tree is generated using the solution of the deterministic expected value problem. The multistage stochastic program for the corresponding tree is then solved in order to yield a lower bound. Since this multistage problem can become very large, Vikas uses a shrinking horizon approach 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. Vikas has shown that this method converges to the rigorous optimum for the case of one uncertain field. Vikas has applied this method to 4 problems. The largest one involved 4 certain and 2 uncertain fields in 8 years. The number of scenarios is 729. A full space formulation would require more than 4 million 0-1 variables. The approximate solution was solved in about 9 hours of CPU time, which incidentally can be reduced to about one hour with trivial parallelization. This solution, which had an expected NPV of $79 million, had a $5.6 million improvement over a deterministic solution.

Scheduling of Batch and Continuous Multiproduct Plants

Student:	**Christos Maravelias (Ph.D. started January 2000)**
New Development	*Novel MILP continuous time model for State-Task Network*
	Novel MILP/CP hybrid method for new continuous time model

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 in multiproduct multistage batch plants. 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. A copy of the reprint describing this work is enclosed.

Regarding Christos he has investigated a new continuous-time MILP model for the short term scheduling of multipurpose batch plants. He has developed a new model that relies on the State Task Network (STN) by Kondili, Pantelides and Sargent (1993) and accounts for resource constraints (other than units), variable batch sizes and processing times, various storage policies (UIS/FIS/NIS/ZW), and accounts for changeover times. Christos has treated the time domain is through intervals of unknown duration, and in which the

continuous events that define the start times of the operations are matched with the start times of the intervals. 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 as is in fact the case in the Ierapetritou and Fludas (1998) model that is based on time events. The idea of decoupling tasks and units is used in the representation of Christos' model. Christos formulated this model first as a hybrid GDP/MILP model, and then reformulated it as an MILP model in which a novel way of expressing assignment and time matching constraints leads to formulations with fewer binary variables. In addition he considered a set of logic cuts leading to tighter LP relaxations. The interesting feature of the model is that it can be solved for profit maximization, cost minimization for fixed demand, and for makespan minimization. The largest problem involved 10 tasks and 14 states in 12 time periods with resource constraints in cooling water, and low and high pressure steam. The model, which had as objective to maximize profit, involved 180 binary variables, 1587 continuous variables and 3067 constraints. CPLEX solved this problem in 2,107 nodes and 63 secs. In that same paper Christos compared his model with the one by Ierapetritou and Floudas showing that his method was at least as fast, and obtained rigorous solutions, which was not always the case in the other model. The manuscript of this work was recently accepted by I&EC Research with excellent reviews. Christos also has extended the model so as to handle due dates.

More recently Christos has also explored the integration of Constraint Programming (CP) in solving the new continuous STN model. The basic idea consists in reformulating the determination of batches and their assignment to equipment with an aggregated MILP model that provides a valid bound. This is then followed with a CP problem with any of the objectives mentioned above. The sequence of iterations is continued by adding special integer cuts until the bounds converge. The MILP formulation is tightened through preprocessing by reducing the range of release and completion times of the batches. Christos has successfully solved several problems with the various objective functions using CPLEX for the MILP and ILOG-Scheduler for the CP part. For problems involving profit maximization reductions of one or two orders of magnitude were achieved. For problems having minimization of makespan as an objective the MILP was typically not solved (even fore a feasible solution) after 6 hours! In contrast the proposed hybrid method required at most few minutes. Christos is currently completing the manuscript on this work.

Uncertainty in the Scheduling of Batch Processes

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

Jayanth, who is scheduled to defend his Ph.D. thesis on March 19, has investigated 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 focused his initial work on flowshop and parallel line scheduling problems, as well as scheduling for new product development. In these cases the major source of uncertainty considered was the duration times.

In his initial work, Jayanth developed a branch and bound procedure for flowshops with zero wait policy in which the key ideas are as followsg. First, for a fixed sequence the analytical expression proposed by Karimi is used to calculate the expected completion time. The property that the expected value of a sum is the sum of expected values (assuming independence) is then applied 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. 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, using 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. Jayanth developed general guidelines and a specific example, which shows that 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 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 been completing the work for 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 showed that it is possible to improve on the conventional two-stage scheduling approach in which a fixed schedule is selected for all scenarios. Jaynath formulated a multi-stage stochastic MILP by considering that the time horizon is subdivided into several subperiods at the end of which rescheduling is performed. In general the large the number of subperiods, the better performance of the schedule. The difficulty with this approach is that the resulting formulation leads to a large-scale MILP, that is expensive to solve. To overcome this problem Jayanth developed a shrinking horizon strategy somewhat similar to the one that was used by Vikas in hiw work. The strategy is based on solving successively two-stage programming stochastic MILPs in which decisions over the subperiods are successively fixed. In this way, one starts optimizing over the entire horizon. After the solution to this problem decisions are fixed in the first subperiod and the horizon is "shrunk" by excluding the first subperiod. The procedure is repeated until only one subperiod is left. 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 shrinking horizon strategy of successively solving two-stage stochastic MILPs, Jayanth obtained solutions that improve the expected profit by 18% over solving the deterministic model once, and 6.5% over solving successive deterministic models, in very reasonable CPU time (~10-20 minutes).

Integration of Product Testing and Planning of Batch Manufacturing Facilities

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

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

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

Christos has recently extended the MILP model for this problem so as to handle variable resource constraints. Specifically, the objective has been to consider that in general more than one resource is available, or that in fact one might purchase additional resources. Christos demonstrated that with the new model the profit could be increased from a loss of $58.9 million to a profit of $241 million, and the time reduced from 80 months to 64 months. A copy of this manuscript is also listed below.

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 avod 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. As a next step Christos intends to automate the proposed solution method in the new version CPLEX 8.0.

Optimal Multiperiod Planning for Catalyst Replacement (DONE)

Research Assistants: Veronique Bizet (started September 2002)

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

Due to the complexity of the process, a semi-empirical model is used that provides reasonable fit with the plant data. This model is used as a basis for developing a multiperiod MINLP model for deciding the optimal catalysts replacement, and operating conditions. The model was applied to problems between 2 and 4 years. Martin implemented the original MINLP model in a GAMS interface that greatly facilitates the use of the model, and 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.

Given the complexity of the original MINLP model, Veronique reformulated the model using concepts of disjunctive programming and logic optimization. This has led to an improved and much clearer MINLP model that can also handle constraints on temperature profiles. Through numerical experimentation Veronique discovered that while DICOPT often finds good solutions, the nonconvexities in the model can lead to suboptimal solutions. In order to try to identify the global optimum, Veronique is investigating a successive optimization strategy that relies on searching over subintervals in the time domain.

Software for MINLP Optimization in Design and Scheduling

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

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

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

Synthesis:

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)*
GDP-DISTILL	GDP Model for the optimal selection of number of trays and feed tray location in distillation columns using tray-by-tray model *(Barttfeld)*

Batch design:

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

Scheduling:

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

Planning:

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

Steinar Hauan's Group

Feasibility and Economics of Reactive Separation Systems

Student: Warren Hoffmaster (PhD, started Jan 2000)

BACKGROUND

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

Many claims have been made as to why these units sometimes perform better than conventional equipment; among them are improved reaction selectivity, higher energy efficiency and lower capital cost. However,

the design and optimization of such multifunctional (or hybrid) units are still more of an art than science. When, for instance, trying to understand how a reactive distillation column really works, several difference views are possible: Are they reactors in which separation occurs, distillation column with chemical reactions or are they neither and require a new set of theories? No matter the answer, there is still a substantial gap in our knowledge in systematically addressing the interactions between fundamentally occurring processes. Consequently, their effect on feasibility and economic potential is far from obvious.

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

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

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

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

PROGRESS

Warren has implemented the first version of the algorithm combining feasible products (in Matlab) with optimal control (in GAMS). The results are described in detail in the enclosed paper and show the pareto trade-off curve between the sum of reactive holdup and the total number of stages in a column for olefin metathesis. As expected, the best results are obtained when the reaction holdup is unevenly distributed between the (potentially) reactive stages. There is further a distinct pattern between the number of non-reactive stages and the total amount of reactive holdup required. Similar case-studies are being performed for systems with strongly non-ideal VLE behavior and the results are also being validated in Aspen. Current work aims at automating the algorithmic steps as well as extending the theory of generalized difference points to explain the results and allow a reduction in the enumerative aspects of the approach.

Agent Systems in Engineering Design and Optimization

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

BACKGROUND

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

His approach assumes that computing capabilities will increase many fold this next decade and that the computing resources will 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. Adesola started less than one month ago and is presently spending most of his time on classes.

Microscale Chemical Synthesis and Sensing

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

(a) improved conversion and selectivity in chemical reactions due to potentially better control of local mixing and heat transfer as well as a surface to volume ratio,

(b) capacity scaleup by device replication and not change of size avoids normal redesign issues when moving from laboratory equipment to pilot plants to production facilities,

(c) improved safety as the small amount of materials and energy present significantly reduces the potential impact of accidents and spill,

(d) clean and cost-effective production of small volumes through the use of cheap, one-time production equipment with no need for downtime and batch cleanup or risk of contamination, and

(e) reduced requirements for physical space and power.

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

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

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

Specific projects:

(a) Microscale Total Analysis Systems

Students: Anton Pfeiffer (PhD, started Jan 2002) and Xiang He (MSc, starting Jun 2003)

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

BACKGROUND

Microfabrication process have enabled manufacture of micro-sized channels, pumps, valves, mixer components and reactors. Integration of these components have enabled the creation of on-chip systems that span sample collection, preparation and analysis of biological materials, drug screening and chemical synthesis. Existing lab-on-a-chip systems tends to consist of relatively few components as the development of each such microscale unit operation continues to require empirical optimization and trial-and-error approaches. Long and expensive development cycles are acceptable for high-volume products where the equipment and process life times are measured in years and a few percent performance improvement translates to large profit. However, the wide variety of biological applications such as genomics, proteomics, therapeutics, diagnostics and a wide-array sensor systems implies the need for many customized designs instead of a few high volume products. Our work aims to create computer tools to aid in the development of customized BioMEMS devices where multiple microfluidic components are tailored to suit individual performance requirements.

PROGRESS

Our current work is directed toward design electrophoretic separation systems. Anton has developed an modular algebraic simulator that is combined with local statements and verified to accurately predict the performance of microscale channel systems. Over the last months, he has performed comparative studies of spiral and serpentine channel arrangements; both compact topologies used in experimental work when minimization of chip area is an objective. As described in more detail in the enclosed paper, the tradeoffs between area, topology and separation performance are complex and depend on both design decisions and fabrication constraints. The simulation based strategy allows us to quickly identify the best topology along with channel layout and physical dimensions.

Current work is directed toward combining rigorous parametric optimization with an iterative method that arrives as the best designs with the input of functional performance specifications only.

(b) A MEMS-based Gravimetric Biosensor

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

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

BACKGROUND

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

There are four major tasks in this project:

(a) fabrication of a CMOS/polymer membrane with integrated capabilities for actuation and capacitive sensing.

(b) chemically specific functionalization of the membrane surface such that target molecules get adsorbed with the highest possible selectivity

(c) creating a clamshell packaging in which liquid samples may be brought in contact with the membrane surface.

(d) computer aided optimization of system parameters – including device geometry, functionalization density and scanning frequencies -- for single membranes as well as arrays of such.

PROGRESS

Mike has been working on tasks (b) and (d) with experimental work on a quartz crystal microbalance reference system and finite element modeling in Femlab. The binding chemistry based on thiols + PEG on gold has been demonstrated for a strongly binding biotin-avidin system. On the theoretical side, Mike has use sensitivity calculations to show that the membrane setup with total surface functionalization is several orders of magnitude more sensitive than current devices in use. Further, the effect of distributed mass-loading has been explored through parametric studies for systems with and without external damping forces (gravity + liquid).

<u>Arthur Westerberg's Group</u>

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

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

and searching parametrically over a and b for the Pareto set. Applying this to the dynamic programming approach for solving, the objectives F2 and F3 become constraints applied at the final time. The search is to find solutions that satisfy these constraints, solving repeatedly for differing values of a and b. However, it is a bit more complicated as these objectives involve expected values. Lifei 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 is preparing a position paper that reviews the very extensive literature on the setting up and solving of stochastic optimization problems, especially those for capacity planning and production scheduling. There are two main approaches to formulating such problem for solving: a math programming approach and an optimal control approach. In this paper we note that one can mix these two approaches along with the dynamic programming approach of our earlier paper to create models that one can solve more rapidly but which we suggest will retain more of the detailed information that is required to make the

correct next decision. His paper describes these ideas and will illustrate them on an example problem. He should be finishing his thesis in May.

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

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

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

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

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

John created, debugged and tested additional agents he needs to find Pareto surfaces for multi-objective problems. He used artificial problems having enormous numbers of local optima for the various objectives, which makes the problem extremely interesting and complex. His testing has shown that collaboration among diverse agents has a remarkable impact. To compare impact he first had to define metrics to indicate how well different agent combinations performed. He uses two. The first one indicates how closely the results from the run are to the best results for defining the Pareto surface he has ever found – both in terms of closeness and coverage (i.e., did he expose the entire tradeoff curve or only a portion of it). A second metric is in how many of the different regions of the best known solution space the run has

placed points. This corresponds to how well he has found the structurally different designs that would be on a Pareto surface. Against these two measures he tried multiple runs of different mixes of different types of agents. The multiple runs were to build up statistical evidence of performance. In one run he ran, for example, only a genetic algorithm (GA) based agent many, many times. In another run he split the function evaluations over both GAs and hill climbers. All combinations one at a time, two at a time, three at a time, etc., of his six different types of agents showed a striking pattern. The more the variety of agents in the mix, the better the results from the testing of them even though each test used the same number of total function evaluations. Over any single agent system, the results are strikingly better.

He ran a test of having the agent population change during the run to see if dynamically controlling the relative mix agents present with time can have an impact. Again, it can have a very large positive impact, suggesting that a learning agent system can be much better than one that does not learn.

Recent progress: John continues to test his algorithms to quantify the impact of collaboration, especially for multi-objective problems. He is introducing constraints and discrete decisions to his artificial problem, with the intent again to test the impact of collaboration on the solving of a well defined but very difficult problem. John, along with Carl Laird – a PhD student working with Larry Biegler, also redesigned and significantly improved the software component that schedules the allocation of resources on a Beowulf cluster. With the explosion in interest in using such clusters, this software will be the basis of a publication.b

Visiting Researchers

Gabriela (Gaby) Mannarino, a post doc from Santa Fe, Argentina, is implementing a personal version of the n-dim modeling environment that one can use on his/her personal computer. N-dim offers a way to organize all the files on a computer that is semantically much more informative than a simple folder hierarchy. In n-dim, one can put an item (a file or another model) into any number of different models. Items in a model can be related through a labeled link. Scripts can be run over these semantically rich structures to effect interesting behavior. We are also defining a "global" version of n-dim that will allow models within personal n-dims to be shared and structured with other people's models.

Erik Ydstie's Group

Distributed Simulation and Control of Process Networks

Students: Vianey Garcia-Osorio
Kendell Jillson

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. Kendell Jillson just joined the group. He started an extensive literature review and will develop new methodology for distributed computing when he comes back after the break.

Modeling and Control Complex Chemical Reactors

Students: Dimitrios Gerorgios
Vianey Garcia-Osorio
Martin Ruzskowski
Marta Duenas Diez

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.

Thermodynamics 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.

Development of New Process Technology for Solar Silicon

Student: Christy White

The PhotVoltaic industry is facing a critical shortage of solar grade Silicon and a large number of manufactures world wide are trying to develop new production technology to meet the demand in a market that continues to grow at a rate of 35-30% annually. We have started and investigation aimed towards the development of new fluid bed decomposition of Silane in a closed reactor, separator system to produce high purity silicon for solar cells. Christy White just joined the group. She will work with SGS on the development of models, process control and optimization technology for this new process.