CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

Lorenz T. Biegler
Ignacio E. Grossmann
Steinar Hauan
Gary Powers
B. Erik Ydstie

Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

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GENERAL NEWS

We are very pleased to welcome two new members to the CAPD: **NOVA Chemicals** and **Petrobras**. The contact with Nova Chemicals, whose R&D facilities are based in Calgary, Canada, will be **Dr. Michel Berghmans**. The contact with Petrobras, whose R&D Center is based in Rio de Janeiro, Brazil, will be **Dr. Euclides Almeida Neto**. We very much look forward to interacting with our new partners.

We are happy to report that **Total** has renewed their membership in the CAPD, despite a reorganization that took place last year that involved divesting Atofina. The contact with Total will be **Dr. Philippe A. Tanguy**, Chaire TOTAL, Ecole Polytechnique, Montreal. Dr Pierre Pestiaux from the Research Center in Gonfreville will be attending the CAPD Annual Review Meeting.

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CAPD e-News. We sent on October 26 our second e-newsletter. As we indicated in our previous newsletter, we will issue a total of four newsletters per year. Two will be the extensive report on projects with preprints in August and January, the two others will be brief e-Newsletters in April and October that will contain short announcements as well as information that we think will be useful to the CAPD members. We would appreciate receiving feedback regarding the e-Newsletter and to the new arrangement.

Erik Ydstie has been invited to give the 2006 Roger W. Sargent lecture at Imperial College. He will also deliver a keynote speech on supply chain systems at the ADChEM meeting in Gremado in Brazil. Erik is also finishing up a new textbook on process control for undergraduate students. The book is co-authored by Profs Karl Johan Astrom, Bjoern Wittenmark and Sten Bay Jorgensen. iLS is in final stages of developing a multi-input single output adaptive predictive controller. It will be beta-tested in April at a power station in Colorado. **Larry Biegler** was a co-organizer (with Frank Allgoewer and Rolf Findeisen) of the International Workshop on Assessment and Future Directions of Nonlinear Model Predictive Control, held on August 26-30, 2005 in Freudenstadt, Germany. **Ignacio Grossmann** organized the Pan American Study Institute on Process Systems Engineering that took place in Iguazu, Argentina on August 16-25, 2005. There were 90 participants from USA, Canada, Mexico, Brazil, Argentina, Chile, Colombia, Venezuela, and Spain. See: http://cepac.cheme.cmu.edu/pasi.htm Ignacio also has become a member of the Strategic Advisory Board of the Institute of Chemical and Engineering Sciences in Singapore, which is located in Jurong Island.

Congratulations to our Ph.D. students who received several awards at the CHEGSA Symposium that took place on October 24-25, 2005. **Yoshiaki Kawajiri** and **Nick Sawaya** received the Symposium Award, and **Carl Laird** and **Anton Pfeiffer** received honorable mentions. Yoshiaki and Carl are students of Larry Biegler, Nick is a student of Ignacio Grossmann, and Anton Pfeiffer is a student of Steinar Hauan**. Congratulations** to **Muge Erdirik** and **Ramkumar Karuppiah** students of Ignacio, and **Israel Owusu**, student of Steinar, who passed their proposal exam in December. Congratulations also to **Brian Baumrucker, and Victor Zavala**, students of Larry, who recently passed their Ph.D. qualifying exams.

It is a pleasure to welcome the following new Ph.D. students to the PSE group: **Anshul Agrawal** and **Parag Jain** from IIT-Dehli, will be working with Larry Biegler. **Mohit Aggarwal**, also from IIT-Dehli, will be working with Erik Ydstie. **Fengqi You** from Tsinghua University will be working with Ignacio Grossmann. Also, the M.S. student **Priyesh Takker** from DJ Sanghvi College of Engineering will be working with Erik Ydstie.

Professor Ostrovsky from the Karpov Institute of Physical Chemistry in Moscow visited Carnegie Mellon in November collaborating with Larry in the area of process flexibility with Professor Luke Achenie from the University of Connecticut. **Sergio Frausto**, Ph.D. student of Vicente Rico at the Instituto Tecnologico de Celaya in Mexico, returned to his country having worked with Ignacio in the area of stochastic optimization for planning of process networks. **Eugenio Bringas,** from the University of Cantabria in Spain visited Ignacio's group from September until December working in the area of global optimization of membrane separation systems for water treatment. **Kristian Nolde,** from ETH, Zurich, and student of Manfred Morari, visited two weeks to collaborate with Ignacio in the area of scheduling and control. **Francesca Pallazzi** from EPFL, Lausanne, and Ph.D. student of Francois Marechal, has joined Ignacio's group for 6 months to work in the area of uncertainty for energy systems, particularly fuel cells.

The **Department of Chemical Engineering at Carnegie Mellon** celebrated its **100th Anniversary** with a one-day symposium on October 26, 2005. On the occasion of this event we compiled a brief history of Process Systems Engineering at CMU. See: http://capd.cheme.cmu.edu/history_pse.html

2006 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on **March 13-14, 2006**. The first day of the meeting will consist of overviews given by Larry, Ignacio, Erik, Steinar and Gary, followed by a discussion with industrial participants, and a poster session by the students. There will also be a dinner that evening at Le Mont Restaurant. The second day is devoted to final year student presentations. Taking into account your feedback from last year which was very positive, we will hold a reception on the evening of March 12 at the Danforth Lounge, University Center. The detailed agenda will be sent very soon. If you have any additional thoughts or suggestions, please let us know.

ENTERPRISE-WIDE OPTIMIZATION INTEREST GROUP

The new special interest group on Enterprise-wide Optimization that is part of the project **"Computational Models and Algorithms for Enterprise-wide Optimization of Process Industries"** and that has been funded by the Pennsylvania Infrastructure Technology Alliance, initiated its activities on October 3, 2005. The participating companies are ABB, Air Products, BP America, Dow Chemical, and ExxonMobil. These companies have supplied case studies that will be undertaken by the EWO faculty and students. The project involves a total of 7 Ph.D. students, and 5 faculty (CMU: **Larry Biegler**, **Ignacio Grossmann**, **John Hooker**; Lehigh: **Jeff Linderoth**; UPitt: **Andrew Schaeffer**). There will be a meeting of this group on **March 15, 2006**, immediately following the CAPD Meeting, to review the progress of the work. Companies who might be interested in joining this group in fiscal year 2006, please contact Ignacio Grossmann. The membership fee to this group is $12,500 for members of the CAPD.

2006 CAPD SHORT COURSE

The short course, ***Process Modeling and Optimization for Process Engineering*** will be offered on **May 31- June 6**, **2006**. In the past we were very pleased with the outcome of this course, as we have had attendees from around the world, both from industry and academia. The course includes the following three modules:

a) Conceptual Design - taught on Wednesday and Thursday (May 31-June 1), with focus on process synthesis, particularly azeotropic and reactive distillation, and design of micro-scale systems.

b) Optimization - taught on Friday and Saturday (June 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 (June 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.

A detailed description of the modules can be found in http://capd.cheme.cmu.edu/shortcourse.html. The course includes extensive workshops where participants obtain hands-on experience with various software packages. Course materials include 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.

VIRTUAL LIBRARY ON PROCESS SYSTEMS ENGINEERING

The Pan American Study Institute on Process Systems Engineering that was organized by **Ignacio Grossmann** took place in Iguazu, Argentina on August 16-25, 2005. The workshop addressed four major areas: Optimization, Process

and Product Design, Process and Supply Chain Operations, and Process Dynamics and Control. A major outcome of the PASI conference was the development of virtual library on Process Systems Engineering covering the four areas. The library consists of the Powerpoint slides of the presentations, background articles, as well as exercises and MATLAB and GAMS computer files for various applications, and a practice exam with solutions. The virtual library can be found in, http://cepac.cheme.cmu.edu/pasilectures.htm

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that the CAPD newsletter is distributed in electronic form. We would appreciate receiving feedback from our member companies of our CAPD website, **http://capd.cheme.cmu.edu.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. We plan to update and modify our website in the next few months. Other websites of interest are Erik's http://mongol.cheme.cmu.edu/, Ignacio's http://egon.cheme.cmu.edu, Larry's http://dynopt.cheme.cmu.edu, Steinar's http://www.andrew.cmu.edu/user/steinhau/ . 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/country.htm** a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada, Mexico and Chile.

CAPD REPORT SERIES

Along with 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

Since the last newsletter, a number of advances have been made in application of large-scale optimization, particularly for dynamic systems. The past few months have seen the following applications.

Some time ago, we proved an equivalence of the optimality conditions for optimal control and our simultaneous nonlinear programming formulation based on orthogonal collocation on finite elements. **Shiva Kameswaran** has recently shown some very useful extensions to this work for path constrained and singular control problems. Two papers, one for path constraints and another for singular control, are listed below.

Dynamic optimization tools, ultimately for on-line use, have been applied that are centered on IPOPT. **Juan Arrieta** has developed NMPC strategies to determine near optimal trajectories for conflict resolution in low-thrust satellites. This is described in a publication listed below. **Victor Zavala** has made strong advances in parameter and system identification for large-scale polymerization processes. Moreover, **Shiva Kameswaran** has applied dynamic optimization to develop ramping strategies for fuel cell power plants. For system identification, **Carl Laird** has expanded the source detection approach for municipal water networks through a novel MINLP strategy that allows specification of a restricted number of contaminant sources. Finally, for periodic adsorption applications**, Yoshi Kawajiri** is currently exploring optimization strategies for Simulated Moving Bed applications, the liquid-solid analog of PSA. In previous work, he has shown substantial improvements in productivity for these systems through an efficient dynamic optimization formulation. Publications that describe this work are listed below.

Enabling Software From Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the interior point nonlinear programming algorithm, IPOPT, in a number of directions. **Andreas Waechter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, based on many of our earlier SQP concepts. In the general purpose framework,

it adopts a sparse decomposition of the KKT matrix, and has been tested on thousands of applications with up to a quarter of a million variables. It has also 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 and the source code can be downloaded from http://www.coin-or.org/Ipopt/index.

Carl Laird and **Andreas Waechter** have migrated the FORTRAN code for IPOPT into an object-oriented code written in C++. The resulting C++ package was released for public distribution last August. The code contains a much simpler interface to modeling environments as well as a more efficient implementation of the algorithm. Finally, the object-oriented code allows for greater flexibility, especially in adopting additional linear solvers and advanced decomposition strategies.

The IPOPT code has already been interfaced to a number of modeling systems including:

- **AIMMS** –This GAMS-like system has a number of extended features including a full graphical user interface for the development of specific user applications. Moreover, it provides exact first and second derivatives and exploits the full capabilities of IPOPT. **Yi-dong Lang** has nearly completed the interface to this system and is currently testing the interface. A similar interface to GAMS is also planned for January.
- **AMPL** – This GAMS-like system is the standard development platform in the Biegler group, has been available for the past two years and can be downloaded from the COIN-OR webpage. It has extensive features for linking to MATLAB and other environments in Unix and Windows. It also provides exact first and second derivatives and exploits the full capabilities of IPOPT.
- **CAPE-OPEN** – IPOPT has been developed under the MINLP object class and has been demonstrated with the CO-Tester. A paper that describes this interface along with a reprint is listed below.
- **MATLAB** – **Claas Michalik** and **Steinar Hauan** developed an IPOPT object that directly links to MATLAB. This object accepts exact first and second derivatives and exploits the full capabilities of IPOPT. Testing of this interface is currently underway.
- **ROMeo** – Recently, **David Ternet** of Simulation Sciences developed an interface between IPOPT and ROMeo, a widely used process modeling and optimization tool for real-time applications. IPOPT is currently being tested and compared with the current OPERA package by **Maame Poku** on a number of large-scale process problems. While ROMeo provides only provides exact first derivatives, it works well with the limited memory BFGS option in IPOPT.

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 updated versions of IPOPT and will be enhanced further by the development of a number of interfaces to optimization modeling platforms including CAPE-OPEN. A paper that describes this work is listed below.

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

In the area of optimization **Nick Sawaya** has continued working in the development of cutting planes for nonlinear disjunctive problems collaborating with Kevin Furman from ExxonMobil. Nick has completed an extensive library of new test problems for the CMU-IBM MINLP open source code project, and has done a theoretical analysis of approximation schemes for nonlinear convex hulls. Also, in collaboration with **Larry Biegler, Gerard Cornjuelos and Pierre Bonami** an open source code for MINLP optimization has been completed that implements the branch and bound, outer-approximation and LP/NLP based branch and bound method. **Lorena Bergamini's** manuscript has been published on the new method for the global optimization for the logic-based OA method that relies on the use of piecewise linear underestimators and avoids spatial branch and bound searches. **Aldo Vecchietti**, has implemented in DICOPT a new option for handling infeasibilities in the NLP subproblems through linearizations in MINLP problems He also continues to work on LOGMIP, a GAMS-based code for disjunctive programming (http://www.ceride.gov.ar/logmip/). **Ashish Agrawal** is completing the writing of his Ph.D. thesis.

In the area of process synthesis **Ramkumar Karuppiah** has developed a novel method for the global optimization for the synthesis of integrated process water systems that must operate under multiple scenarios. The proposed method relies on a decomposition scheme that relies on Lagrangean relaxation. **Jose Caballero** has completed a manuscript on the synthesis of heat integrated and thermally integrated distillation columns for which he has proposed a novel solution approach that allows him to obtain the entire range of designs, from no heat integration to full thermal integration. In a joint collaboration project with BP, **Carlos Mendez** has performed the integrated optimization of refrigeration systems with the superstructure optimization of a crystallization process for the separation of paraxylene. In a joint collaboration project with **Mike Domach, Soumitra Ghosh** has applied concepts of the Analytical Hierarchy Process by Setty for screening of NMR analytes for determination of metabolic flux maps.

Vikas Goel, who has joined ExxonMobil**,** completed his manuscript describing a Lagrangean based branch and bound method for solving multistage stochastic programs in which the scenario trees are dependent of the design decision. He applied this technique to the planning of gas fields. **Bora Tarhan**, has addressed the problem of optimal planning of process networks with uncertain yields and in which time varying uncertainties are considered as well as possibility of installing pilot plants for reducing uncertainty. He has developed a formulation and solution method that represent an extension of the work of Vikas Goel. **Sergio Frausto**, has worked on a two-stage programming model for strategic supply chain with uncertain demands that are described by continuous distributions. His solution method relies on sampling and decomposition. **Muge Erdirik** completed her manuscript in the area of simultaneous planning and scheduling for continuous multiproduct plants, and has started to address a multistage planning and scheduling problem that was supplied by Dow. She has obtained encouraging results for an STN based aggregated planning model. **Minhwan Park** and **Fernando Melle** have developed cost models that reflect different contracts for supply chain optimization problems for which they used a disjunctive programming approach, and applied them very effectively to short and long term planning problems. **Carlos Mendez** is currently revising a very comprehensive manuscript that provides a review of the area of short-term batch scheduling. Also, for the refinery scheduling and blending problem we developed sufficient conditions for the convergence of the MILP. **Pedro Castro** has been investigating various formulations for multistage problems with parallel units, including a novel RTN MILP formulation. Also, in conjunction with Carlos Mendez and ABB (Iiro Harjunkoski and Marco Fahl) he has developed a sequential decomposition strategy for complex multistage batch plants. Finally, in collaboration with **Antonio Flores-Tlacuahuac** from Mexico, he has developed a combined scheduling and dynamic optimization model for a multiproduct CSTR reactor in order to account for optimal control in the transitions.

Steinar Hauan's Group

Anton Pfeiffer and Xiang He have completed their work on a system-level simulation engine for microscale Lab-on-a-Chip (LoC) systems. The approach is based on topological decomposition where the LoC is represented in a graph, the driving forces solved as a resistor network and the individual unit operations solved in a sequential modular fashion using reduced order models. This sets the stage for the design of integrated and multifunctional LoC units.

Mike Bartkovsky (experimental focus) and Jane Valentine (modeling focus) continue their work on MEMS-based biosensors. Mike has spent most of the Fall semester developing the experimental procedures by which one may reliably measure and quantify the vibration of the mechanical structures and thus extract necessary physical parameters such as elasticity, flex and damping coefficients. Jane has started using her reduced order analytic vibration model to design integrated sensing arrays, i.e. systems where multiple species may be targeted for detection with a single sensing element.

Murni Amhad has moved several steps toward the systematic generation and evaluation of flowsheets for protein separation by liquid-liquid extraction. As expected, the presence of recycle streams may cause iterative calculations for multi-stage systems to fail due to the highly sensitive thermodynamic calculation routines as well as the relatively small feasible regions for liquid-liquid phase separation. The goal is to move to an optimization based approach this upcoming semester.

Israel Owusu -- working on asynchronous approaches to distributed Enterprise Resources Planning -- has implemented a system for solving multisite planning and scheduling problems in a distributed fashion. Initial case studies indicate that even in capacity constrained situations, iterative demand partitioning strategies can give reasonable overall solution quality while keeping the computational complexity out of the exponentially dominated region. More general strategies for information sharing and cross-site coordination are being explored.

Scott Turnberg studies the optimal design of combined reaction-separation systems using feasible regions. The approach is based on previous work by Warren Hoffmaster, but has been extended to analysis of systems with disjoint product composition regions separate by bifurcations in the interior of the composition diagrams. Current work aims at developing the basis for feasibility analysis in systems with multiple independent chemical reactions with the goal of identifying multiproduct reactive separation units.

The Beowulf computer cluster has been very stable this semester and the average usage has been high. The next generation cluster room --relevant for the upcoming Doherty Hall renovation -- has been designed and will be expanded to also house a cluster for the environmental group in the department.

Congratulations! Xiang He and Israel Owusu have passed their PhD proposal exams.

Gary Power's Group

Professor Gary Powers and Masters student Denny Jacob have completed a study testing the validity of procedures for the hydro-testing of piping systems for off-shore oil platforms. Hydro-testing is done to detect leaks in piping systems due to defective welds, valve seals, etc. In this study, Mr. Jacob constructed a modular logic model of the steps and equipment in hydro-testing procedures used by the American Petroleum Institute and numerous construction companies. The models included failures of the sensors, equipment, humans and procedures. The system model was verified against system specifications using the model checking system SMV, Numerous faults that have occurred in testing off-shore piping systems were detected as well as several faults that have not occurred yet. Case studies were performed to indicate how the hydro-testing procedures could be improved. Data from current testing procedures will be gathered to validate the models and suggested improvements.

Erik Ydstie's Group

The Ydstie research group works on developing advanced modeling and control system methods for chemical processes. The work is distributed along two distinct axes. The first axis concerns how to use process physics and passivity based control theory to develop distributed simulation and control methods for chemical process networks. We are especially interested in developing methods that integrate physics, computation and communication in coherent and stable ways. The second axis is based on the idea of incorporation learning and adaptivity in control and optimization. We are especially interested in studying how we can learn and adapt simple representations of optimal control (discrete and continuous decision making) in complex systems.

Christy White has developed an efficient way to represent and model particulate processes. She has developed inventory control approaches for such processes and a general approach for state and parameter estimation. The problem she is working on is motivated by the direct reduction Saline to form high purity silicon for the photo voltaics industry.

Kendell Jillson has developed very efficient methods for how to model and integrate very complex process networks in a stable manner. He has developed methods that show how such systems can be designed to be self-stabilizing and self optimizing. He is currently adapting the modeling paradigm so that it can be used to represent bio-processes.

Eduardo Dozal has developed a new method for real time optimization which can be used to solve complex problems in non-convex optimization. The method works by filtering out "surface roughness" and embedding the high dimensional problems in a low dimensional input output representation of the system to be optimized.

Yuan Xu joined the research group in January. He is working on stability analysis, distributed simulation and batch chemical control. He uses passivity based methods and integrates it with non-equilibrium thermodynamics. His application domain is the carbothermic reduction of aluminum oxide to form aluminum.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

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

As a result of several generations of Ph.D. students, we now have a number of very efficient NLP algorithms including rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. As described above, the most recent incarnation is IPOPT, with continuing development by Andreas Waechter. This code has become a core algorithm for many of the research projects described below. Three reprints that describe the basic algorithm as well as the convergence properties are listed below. In addition, Carl Laird has applied IPOPT and the AMPL interface to develop a novel source detection strategy for municipal water networks as an important application for barrier methods. This optimization problem is developed to detect attacks on networks and to determine optimal control and remediation strategies. Such networks are typically over several hundred to many thousands of nodes and require the incorporation of both spatial and temporal behavior. This difficult problem was reformulated as a DAE system with time delays. Moreover, because the hydraulic equations could be decoupled from the species mass balance, a novel preprocessing strategy renders the nodal constraints to be *linear* and the resulting problem can be solved easily using our simultaneous optimization strategies for dynamic optimization (see below). By exploiting the structure of these networks, discretized problems that represent actual municipal networks with up to 300,000 variables could be solved in only a few CPU seconds. More recently, this approach has been extended, by using an MIQP strategy, to a more robust one that promotes unique solutions. Using an efficient pre-processing step, small subproblems can be derived and attack scenarios can be identified more precisely and efficiently. This approach is described in a publication below. Finally, Carl spent the past summer with Andreas Waechter at IBM to complete development on the next version of IPOPT. Designed in C++, this code is object oriented and flexible to deal with a wide variety of linear solvers, new barrier algorithms, and a variety of globalization strategies and decomposition approaches. Moeover, as noted above, the new code provides a much easier interface to modeling environments. Carl is currently expanding the IPOPT code to accommodate multiperiod problems. These are essential to deal with process optimization under uncertainty and have a structure that can be decomposed through Schur complements and can be completely parallelized on distributed memory machines. Carl has obtained some preliminary results with this decomposition that validate these properties. Detailed results of this implementation will be discussed in the next newsletter.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: Juan Arrieta (Ph.D. started Fall, 2002)
Brian Baumrucker (Ph.D. started Fall, 2004)
Prof. Ricardo Perez (Pontifical University of Chile)

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 recently completed his Ph.D. and has accepted a position with United Technologies. In his research, he has incorporated the MPEC formulation into the IPOPT code, now called IPOPT-C, 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, dynamic systems with switching conditions, such as overflows and phase disappearance in distillation columns and metabolic network systems. For the latter, we have considered parameter estimation problems for dynamic fermentation systems for wine production. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies.

Current work by **Juan Arrieta** deals with modeling and optimization of dynamic biological systems that are based on cellular models. Such systems are large-scale extensions of MPECs. Moreover, they have interesting modeling features since state dependent constraint functions with discontinuities also need to be treated through MPEC formulations. Moreover, **Brian Baumrucker** recently passed his PhD qualifier and is currently considering the development of good MPEC formulations that model discrete decisions. He is currently working with the ROMeo real-time optimization package and is exploring formulations for complementarity conditions within real-time optimization models. In particular, he has shown that penalty-based NLP formulations have worked very well on these models. Moreover, with these formulations, one is able to decouple problem-specific optimization algorithms from the optimization model and rely on general purpose optimization solvers. In addition to the ROMeo comparison described above, he is investigating complementarity formulations in distillation columns with mass transfer limitation.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Researchers: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
Shivakumar Kameswaran (Ph. D. started Fall, 2001)
Victor Zavala (Ph.D. started Fall, 2004)
Yi-dong Lang (Jiansu Research Institute, Nanjing, China)
Prof. Antonio Flores Tlacuahuac (Unversidad Iberoamericana)

The topic on simultaneous solution and optimization strategies for large-scale, dynamic optimization problems incorporates a number of projects. In the past, 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. 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. Prof. Antonio Flores, a sabbatical visitor from the University of Iberoamericana, has demonstrated the advantages of this approach on a number of challenging polymerization processes. Moreover, he has recently extended this to consider the application of global optimization strategies for these problems. A paper that describes this approach is listed below. Moreover, the following research projects are currently being addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization, one based on reduced space and one on full space. 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 ESO interfaces 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. Further reformulations of this system, using a simple partitioning strategy, have led to an optimization problem that is much better conditioned and can now be solved in only about 1000 CPU secs. Finally, DynoPC has been extended to solve the dynamic optimization problem for moving finite elements. A paper that describes *DynoPC* and the moving finite element approach is listed below.

Second, we have been using IPOPT in a full space framework linked to the AMPL modeling environment. As detailed in many of the studies listed below, this framework has been extremely powerful and flexible in solving a wide variety of problems. We are currently adopting a MATLAB framework and have coupled it with the AMPL modeling language. Domain specific prototypes have already been developed and work very well.

Consistency and Convergence of Simultaneous NLP Formulations for Dynamic Optimization

Does the solution of the discretized NLP converge to the solution of the original optimal control problem? What are the particular problem classes and assumptions for which this can be shown? This has been an interesting and long-standing research problem. Back in 1989, we have developed some consistency results based on the work of Reddien for Gauss collocation schemes. In addition, Lagrange multipliers from the KKT conditions have a direct relationship to adjoint variables from the Euler-Lagrange equations. However, more powerful convergence results are difficult to show and usually apply only to well-conditioned linear-quadratic control problems. Nevertheless, despite limited convergence results, very good performance is usually obtained with simultaneous optimization strategies.

Recently, Shiva has revisited some of the theory in order to derive properties for Radau and Lobatto collocation. Both of these methods (while of lower order) tend to behave much better than Gauss collocation. We have recently derived order conditions for these methods and have related their convergence properties to the more general class of boundary value solvers. Moreover, these have been verified by a number of example problems. Currently, Shiva has extended this approach to the solution of singular control problems. These features lead to ill-conditioned KKT matrices, nonunique solutions and possible failure of the NLP solver. Based on the convergence analysis, we are refining several regularization formulations that will regularize the KKT matrix and provide a consistent theory for more general optimal control problems.

Nonlinear Model Predictive Control Strategies

Through collaborations with D. Subramanian and T. Samad at Honeywell, Inc. Arvind Raghunathan had been pursuing an important research problem on conflict resolution of aircraft trajectories. Given a set of aircraft with starting points, destinations, protection zones and obstacles, what are the optimal trajectories that lead to the best performance or minimum fuel consumption? Moreover, detailed flight models are employed that limit the maneuverability of these aircraft. This problem leads to a nonconvex dynamic optimization problem. Moreover, protection zones lead to disjunctive constraints that have been modeled through convex hull formulations. The resulting problems are discretized using collocation on finite elements and solved using IPOPT.

Our current work extends these off-line strategies to on-line nonlinear model predictive control (NMPC). Here only partial solutions are considered for the aircraft trajectory and efficient NLP solutions are required in order to guarantee on-line performance and stability. Juan Arrieta has recently developed two prototype formulations: an NMPC strategy based on a detailed NLP solution and an MPC strategy based on solutions of QPs. Both of these strategies have demonstrated efficient partial solution strategies that allow conflict free flight in the face of many aircraft and obstacles. In particular he has shown that the NMPC strategy does not suffer from large deviations from the optimal trajectory in the nominal case; it has handled pop-up threats and incorporates limitations due to radar ranges. Juan has also extended this approach to a number of more complicated aerospace models including satellite trajectories and NMPC variations of these trajectories. His recent work has shown that our approach generates optimal solutions significantly faster than competing methods. Two papers that describe the approach are listed below; one deals with NMPC applied to unmanned aircraft, while the second deals with satellite trajectory optimization and updating these trajectories with NMPC to compensate for disturbances.

Finally, the NMPC strategy is also being extended to large-scale models for polymerization processes. In a project funded by ExxonMobil Chemicals, **Victor Zavala** has begun to develop multi-stage dynamic optimization problems for grade transition and defouling operations; he recently passed his PhD qualifying exam. As the first step, he has developed a detailed reactor model of a polyolefin reactor. The model includes a complete kinetic description and is used for parameter estimation using actual process data. Using AMPL and IPOPT, Victor has extended this model to multiple data sets as well as EVM problems (where errors in both inputs and outputs are considered). Applying this approach to a large number of data sets, Victor was able to estimate kinetic parameters quite well; the scatter of the data was reduced by an order of magnitude, compared to previously fitted models. This approach was presented at the recent AIChE meeting and a paper will be included in the next newsletter.

Large-Scale Optimization for Fuel Cell Models

Researchers: Cong Xu (Ph.D. completed Spring, 2005, joint with Prof. M. S. Jhon)
Shivakumar Kameswaran (Ph. D. started Fall, 2001)

Cong Xu recently completed his PhD and is doing postdoctoral studies. For his thesis project, he has been investigating optimization problems arising in fuel cell applications, including Direct Methanol Fuel Cells (DMFCs) and Hydrogen PEM fuel cells. In particular, he has extended simple DAE models for fuel cells to consider optimal flow patterns and minimization of contamination effects due to membrane crossover, and he has extended these models to consider sensitivity and optimization calculations. In particular for DMFCs, Cong Xu and Peter Follmann have compared and critically assessed several literature models and have explored the crossover phenomenon. By applying our dynamic simulation and optimization tools, they were able to develop dynamic feeding strategies for these systems that greatly reduce contamination due to methanol crossover. These systems have been modeled and optimized with a variety of FORTRAN, MATLAB and MAPLE-based tools, such as OCC. The results show that the optimal design of DMFCs can be achieved without pulsed operation. Here crossover is significantly reduced and the power density is correspondingly increased. The efficiency of these processes can also be improved through flowsheet optimization strategies as well as heat integration of the process units. This approach is based on conventional flowsheet optimization schemes within Aspen/Plus along with simultaneous optimization and heat integration strategies. The application to fuel cell based processes leads to interesting trade-offs between the fuel cell, the rest of the flowsheet and the heat recovery system.

Dynamic optimization has also been applied by Shiva Kameswaran to develop ramping strategies for fuel cell power plants. In a project funded by Fuel Cell Energy, Inc. and DOE, Shiva has demonstrated significant improvements in maintaining power levels with more energy efficient operation. Using AMPL and IPOPT, he has incorporated detailed models of the entire power plant and has demonstrated this approach both for parameter estimation and optimal control. This approach was presented at the recent AIChE meeting and a paper will be included in the next newsletter.

Optimization and Control of Periodic Adsorption Processes
Student: Yoshi Kawajiri (Ph.D. started Fall, 2003)

In her Ph.D. thesis, Ling Jiang developed an efficient optimization strategy for Pressure Swing Adsorption (PSA) systems. Working with Grant Fox at Air Products, she applied rSQP as well as 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. *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. Finally, this work has been applied to complex PSA systems for the separation of high purity hydrogen from refinery gases.

These successes have led us to consider applications in Simulated Moving Beds (SMB), the liquid analog to PSA. Simulated Moving Bed (SMB) chromatography was developed in the 1960s as a realization of continuous chromatographic separation. Since then, SMB has been gaining attention in food, sugar, and petrochemical applications. In more recent years, SMB has been recognized as an attractive technology for enantiomeric separations in the pharmaceutical industry. An SMB system is realized by connecting multiple columns in a cycle. The feed and desorbent are supplied continuously between columns, and at the same time extract and raffinate products are withdrawn. Counter-current operation is "simulated" by switching these inlet and outlet streams intermittently in the direction of the liquid flow. As with PSA this system is characterized by a Cyclic Steady State (CSS), where the concentration profiles in the columns change dynamically but repeat the same pattern in every cycle.

Over the past two years, **Yoshi Kawajiri** has been investigating efficient optimization strategies for these systems. Here optimization methods can be based on the single-discretization approach to discretize the Partial Differential Equations (PDEs) only in the spatial domain and then integrate the resulting Differential Algebraic Equations (DAEs) in time. On the other hand, the full-discretization approach discretizes the PDE both in time and spatial domain, leading to a large-scale Nonlinear Programming (NLP) problem. Yoshi has compared both approaches and found that the latter approach has shown tremendous improvements in the productivity of SMB systems. Moreover, these were obtained almost two orders of magnitude faster than with the single discretization (sequential) method used in gProms. The approach was applied to optimization of SMB systems with steady and time-varying feeds (i.e., PowerFeed), both for linear and nonlinear isotherms. This efficient approach also allows us to consider the design and control much more complex SMB systems. In particular, Yoshi has developed a superstructure SMB system that allows for the optimization of a number of novel, recently reported designs, as well as some new ones. The superstructure leads to a well-defined and easily solved problem formulation. Preliminary results have yielded innovative designs with improvements in productivity. A conference paper that describes this approach is listed below. More extensive results are now being compiled for a paper distributed with the next newsletter.

Ignacio Grossmann's Group

Open-Source Code for MINLP Optimization

New developments: **Open source code that integrates various methods has been completed**

Post-doctoral fellow: **Pierre Bonami (Tepper)**

Collaborators: **Larry Biegler, Gerard Cornjuelos (Tepper), Francois Margot (Tepper)**

Students: **Nick Sawaya, Carl Laird**

This is a project in collaboration with researchers at IBM (Andreas Wächter, Andy Conn, Joantahn Lee, Andrea Lodi). The main objective has been to develop open source code for solving MINLP problems.

In the first phase of the project we have restricted ourselves to solving MINLP problems that have a convex relaxation. The postdoctoral fellow Pierre Bonami has developed a code that solves MINLP problems with the NLP-based branch and bound, outer-approximation and the LP/NLP based branch and bound method. Both the outer-approximation and the LP/NLP based branch and bound method are based on our previous work (Duran and Grossmann, 1986; Quesada and Grossmann, 1992). There are, however, three important issues. First, the implementation provides a single computational framework for the three methods. When no linearizations are performed the method reduces to NLP-based branch and bound. When linearizations are performed this can be done by completing the LP-based branch and bound at each cycle followed by the NLP subproblem. When the LP-based branch and bound is not completed, the NLP subproblems can be solved at intermediate nodes, for instance at integer feasible nodes like in the original Quesada and Grossmann method. Second, the LP/NLP based branch and bound has been extended to a more general branch and cut scheme in which NLP subproblems do not have to be solved at only integer feasible nodes, but they can be solved at any intermediate node. For convenience we have termed this method "hybrid" as it represents an in-between NLP-based branch and bbound and outer-approximation.

Third, the code makes use of the following open source codes: IPOT from Andreas Wächter and Larry Biegler, and CLP or CPB from the COIN-OR library.

Pierre has tested his code with close to two hundred test problems. Nick helped to build most of the convex MINLP problems of this library, which include batch design, retrofit planning, layout and trim loss problems. Carl Laird also contributed with some water contamination problems that involve a large number of continuous variables. The test problems are available in the webpage: http://egon.cheme.cmu.edu/ibm/page.htm The performance of the open source code was compared with both SBB, the branch and bound code in GAMS, and DICOPT, the outer-approximation method that is also available in DICOPT. The computational results on a representative subset of 38 the 200 problems showed the following trends. DICOPT solved 20 of the 38 problems the fastest and in less than 3minutes. Among these was a retrofit planning problem with 576 0-1 variables, 2720 continuous variables and 4980 constraints. The hybrid method (i.e. branch and cut) proved to dominate for the remaining 18 problems in terms of speed and successful completion. Among these was a problem with 14 0-1 variables, 107,222 continuous variables, and 107,209 constraints. It is also interesting to note that the hybrid method always dominated the NLP-based branch and bound as well as the open-source outer-approximation method. A paper reporting this project as well as the numerical experiments has been completed and is available in the list at the end. An additional paper that will concentrate on the large set of test problems with an explanation of them is being prepared by Nick, Carl and Pierre. Our next major step in this project will concentrate on handling nonconvexities in an "ad-hoc" manner, that is without performing rigorous global optimization.

Algorithms for Nonlinear Disjunctive Programming

Student:	**Nicolas Sawaya [Ph.D., started Jan02]**
Visitor:	**Lorena Bergamini [Ph.D. Jan 03]**
Research collaborator:	**Aldo Vecchietti [Researcher at INGAR]**
New Developments:	**Rigorous approximation for nonlinear convex hull reformulation**
	New option in DICOPT for infeasible NLP subproblems

Nicolas Sawaya

The 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. A major objective in Nick's work has been to develop effective cutting plane methods for linear GDP problems. The other objective has been to develop an integrated framework for solving nonlinear GDP problems.

The first major step in Nick's research work was to develop a solution method for linear GDP problems that relies on cutting planes, and that can be embedded within a branch and cut algorithm. The major steps of the algorithm are to first solve the big-M relaxation. Next, we formulate and solve a separation problem in which we minimize the difference between a 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 one can derive a cutting plane. The derivation of successive cutting planes continues until the improvement in the lower bound of the big-M model with the cutting planes lies within a tolerance. The idea is then to switch to a branch and bound method. Nick has developed a theoretical derivation of the cutting planes for the 1, 2 and infinity norms based on the use of subgradient optimization. Nick applied his cutting plane technique to three major problems using the infinity norm. The first is the strip packing problem that consists of fitting a set of rectangles in a roll of fixed width in order to minimize its length. The largest problem that Nick solved involved 21 rectangles. The convex hull formulation is significantly larger than the big-M model (5272 vs 1072 constraints, 4244 vs 884 continuous variables; both have 840 0-1 variables). The big-M formulation required 1 416 137 nodes and a CPU-time of 4093 with CPLEX 8.1. The convex hull formulation required 968 652 nodes in a time limit of 10 800 secs in which the problem was not solved to even feasibility. In contrast with 60 cutting planes the number of nodes was reduced down to 28611 nodes and 79

seconds! It should be noted that these times include the times for solving the separation problem. Nick also solved 10 process retrofit problem, and extension of a model that Jennifer Jackson formulated, and he also addressed a job-shop scheduling problem with up to 10 jobs and 8 stages. The cutting plane technique was not very helpful in both cases, although in the retrofit problem it did improve substantially the performance of the big-M reformulation.

Nick has also been investigating the use of cutting planes for solving nonlinear disjunctive problems. He has considered as a first step nonlinear GDP problems that are reformulated as big-M MINLPs and solved them through branch and bound. Nick has recently tested this method on a retrofit planning problem. The convex hull reformulation involved 2218 constraints, 1348 continuous variables and 282 0-1 variables. In contrast the big-M model only involves 1648 constraints, 706 continuous variables and 282 0-1 variables. The convex hull formulation was solved in 711 secs enumerating 1563 nodes. The big-M formulation was stopped after 3 hours enumerating 48816 nodes. The NLP relaxations were 2916 and 8088.9, respectively. With the proposed cutting plane method, using the infinity norm, the NLP relaxation of the big-M was increased to the one of the convex hull with 209 cutting planes. In that way the number of nodes was reduced to 1215, and the required time to 341 secs (including 103 secs for the cut generation). Thus, the proposed cutting plane led to significant improvements. Nick is currently applying his cutting plane method to different solution methods for GDP (e.g. logic based OA, disjunctive Branch and bound).

As indicated in the previous newsletter a n important issue is how implement the constraint $\lambda g(\nu/\lambda)\le 0$ for the case when λ goes to zero and when g is nonlinear and convex. In our previous work we had used the simple approximation $(\lambda+\varepsilon)\, g(\nu/(\lambda+\varepsilon)\le 0$. This however can give rise to problems depending on how ε is selected. The main problem here is that if ε is set too small there are problem with accuracy. If ε is somewhat large then if a disjunct term does not apply and the inequalities are violated it may make the approximation infeasible. Nick had proved that a rigorous approximation that avoids both problems is given by $(\lambda_{jk}+\varepsilon)g_{jk}(\nu_{jk}/(\lambda_{jk}+\varepsilon))\le \max_{\nu_{jk}\in(0,U_{jk})}(\max\ (\varepsilon g_{jk}(\nu_{jk}/\varepsilon),\ \varepsilon g_{jk}(\nu_{jk}/(1+\varepsilon))))$, where the basic idea is that the term on the right hand side represents a relaxation that can be made arbitrarily small. Since the constraints are convex, the maximization on the right hand side can be computed by evaluating the functions at the extreme points for each inequality which are few for sparse problems. In this way the actual expression can be simplified to, $(\lambda_{jk}+\varepsilon)g_{jk}(\nu_{jk}/(\lambda_{jk}+\varepsilon))\le \max\ (\varepsilon g_{jk}(0),\ \max_{\nu_{jk}\in(0,U_{jk})}\varepsilon g_{jk}(\nu_{jk}/(1+\varepsilon)))$. Nick however, also found an alternative expression given by $(\lambda_{jk}+\varepsilon)(g_{jk}(\nu_{jk}/(\lambda_{jk}+\varepsilon))+g_{jk}(0)(\lambda_{jk}-1))\le 0$, which is easier to implement. Nick was able to show that in fact the latter expression is superior compared to the first one in terms of accuracy, under most circumstances. The exceptions rarely hold true. Nick has successfully tested this approximation scheme in several examples (analytical, process network, safety layout) using values of $10^{-7}\le\varepsilon\le 10^{-4}$. The results have shown that very good approximations are obtained with both methods, although the second approximation outperforms the first. Based on input by Kevin Furman from ExxonMobil, Nick has been considering the alternative convex expression $((1-\varepsilon)\lambda_{jk}+\varepsilon)g_{jk}(\nu_{jk}/((1-\varepsilon)\lambda_{jk}+\varepsilon))-\varepsilon g_{jk}(0)(1-\lambda_{jk})\le 0$ which not only circumvents the infeasibility that arises in the original Grossmann & Lee expression, but, when $0 < \varepsilon < 1$, it is exactly equivalent to the (true) CH expression at $\lambda = 0$ or 1, regardless of the value of ε within that range. This scheme is being examined by Nick in collaboration with Kevin.

Lorena Bergamini

Lorena, a Ph.D. student from INGAR in Argentina working under the direction of Pio Aguirre and who spent one semester with us, developed a new deterministic algorithm for the global optimization of process networks that are formulated as Generalized Disjunctive Programs and that involve nonconvexities. The global optimization algorithm relies on the use of piecewise MILP approximations (no spatial branch and bound search). Also, the method is based on the Logic-Based Outer Approximation (OA) algorithm developed previously by Metin Turkay and that overcomes difficulties related to singularities that are due to zero flows. The method developed by Lorena is capable of handling nonconvexities, while rigorously guaranteeing the global optimality of the synthesis of process networks. This is accomplished by constructing a master problem that is a valid bounding representation of the original problem, and by solving the NLP subproblems to global optimality. Lorena assumed that the functions involved are sum of convex, bilinear, and concave terms. In order to rigorously maintain the bounding properties of the MILP master problem for nonconvex problems, piecewise linear under and overestimators for bilinear, and

concave terms are constructed over a grid with the property of having zero gap in the finite set of points. The set of these approximation points are defined over subdomains defined by bounds of variables and solution points of the previous NLP subproblems. For bilinear terms, the convex envelope by McCormick is used. Disjunctions are used to formulate the convex envelope in each subdomain, and the convex hull of these disjunctions is used to provide the tightest relaxation. Linear fractional functions are treated in a similar way. Piecewise linear subestimators replace the concave terms. The NLP subproblems are also solved to global optimality using a reduced MILP master problem. Since the NLP subproblems are reduced problems, involving only continuous variables related to a process with fixed structure, the variable bounds can be tightened thereby enhancing the underestimators. Lorena has applied this algorithm on a number of different problems. For instance, the algorithm has been applied in a process network problem that originated in an internship of Sangbum Lee at Eastman Chemical and that involves 17 Boolean variables, 973 continuous variables and 725 constraints. The algorithm required 5 minutes, while BARON could not solve the problem within 15 minutes. Lorena has completed a manuscript on this work which is enclosed as a reprint.

Aldo Vecchietti: LOGMIP and DICOPT

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 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 (e.g. $g(x) \leq 0 \Rightarrow f(x) \leq 0$) can be systematically converted in the form of disjunctions. The intent is also to be able to accommodate hybrid models that are partly expressed as disjunctions and partly as equations in algebraic form.

Aldo has completed in LogMIP the definition of disjunctions over sets and subsets. The conditional statement operator WITH in conjunction with other operators: relational operators (<, <=, =, >, <=), logical operators (and, or) and sets operators (ord, card, in) or using a subset definition are used to control de disjunction's domain defined over a set. As for the propositional logic, the special constructs ATLEAST, ATMOST, EXACTLY are defined to specify that the sum over a subset of variables with a given cardinality is at least, at most or equal to one. Also, LogMIP can now accept logic propositions in symbolic form without the need of translating them into linear inequalities.

For solving linear disjunctive/hybrid problems LOGMIP can automatically generate the convex hull relaxation and big-M transformation for linear problems. Aldo has implemented LogMIP in the IDE version of GAMS and tested it with several problems that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. The latter has yielded very impressive numerical results. Aldo found that the big-M formulation of the retrofit planning problem takes about 1745 nodes with OSL, while convex formulation through LOGMIP only requires 9 branch and bound nodes!. For solving nonlinear disjunctive/hybrid problems Aldo has also automated the logic-based OA algorithm by Metin Turkay, which is suitable for nonlinear GDP process network problems. Work is under way to implement the reformulations for nonlinear GDPs. The LogMIP Website is now also available, http://www.ceride.gov.ar/logmip/. The Website includes now some explanation about LogMIP, the User's manual, solvers and examples downloads, references and links.

Aldo has added a capability in DICOPT for handling more effectively infeasible NLP subproblems. In the current version an integer cut is simply added if the NLP is found to be infeasible. This is often very ineffective as the integer cut is quite weak, especially as the dimensionality of the 0-1 variables increases. What Aldo has done is to allow the addition of linearizations of the infeasible NLP subproblems. When using a solver like CONOPT the linearizations will be derived at a point where the infeasibility is minimized. This option is rigorous for the case of convex MINLP problems. For nonconvex problems there is the risk of cutting off optimal solutions. To solve problems in GAMS with linearization in infeasible NLPs the following option must be defined: infeasder 1. By default infeasder is 0. In this case DICOPT runs like the previous version (just with the integer cut with NO linearization on the infeasible points). This new option has shown to significantly improve the performance of DICOPT in several problems, which often did not converge with the old version. This performance has also been verified by Nick Sawaya on several difficult convex layout problems that tend to produce infeasible NLP subproblems.

Modeling of Hybrid Systems and Mixed-integer Programs

New developments: **Completing Ph.D. thesis**

Students: **Ashish Agarwal [Ph.D., started Jan 02]**

The initial objective of Ashish's project was to develop a new hybrid systems framework for modeling supply chain networks. The basic idea in Ashish's project has been 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. Ashish developed a representation based on automata than can be systematically transformed into one with finite states, then to a disjunctive programming model, and finally into a mixed-integer linear program. In this way an important accomplishment is that one can systematically derive the mixed-integer linear programming model describing the supply demand optimization network problem. Ashish has tested the model formulation on a small supply chain optimization problem demonstrating that the model can be expressed in very compact form. Ashish has completed a manuscript describing this work.

Over the last year, with the collaboration of Professor Bob Harper from Computer Science, Ashish has been investigating the use of Type Theory as a systematic formalism based on logic for proving correctness of formulations for mathematical optimization. The basic idea in type theory is to rigorously define the different variable and operator types using logic constructs to ensure that all transformations of data, variables and equations are "well-formed." In this way one can use such a representation to define mappings as is for instance the case of the reformulation of generalized disjunctive programs to mixed-integer linear programs. Furthermore, one can use type theory as a basis for developing software that has a strong foundation, and that is more likely to be free of errors. Ashish has applied this formalism to generalized disjunctive programming problems for transforming them automatically into MILP models. This has required a sophisticated theoretical development based on type theory that in turn he has used as a basis for software development. Asish has used the language ML for developing the software and has demonstrated the application to several GDP models that are derived from the automata representation, and that can be automatically converted into MILP problems. Ashish is in the process of finishing his Ph.D. thesis and of writing the corresponding papers.

Optimal Synthesis of Integrated Process Water Systems

New developments: **New algorithm for multiscenario water problems with uncertainty**
New optimization algorithm for membrane systems

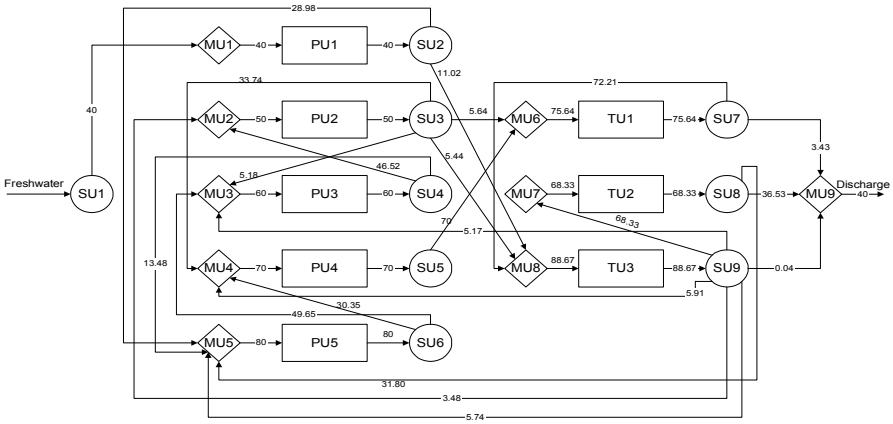
Students: **Ramkumar Karuppiah [Ph.D. started Jan 04]**
Visitor: **Eugenio Bringas (Univ. Cantabria, Spain, Sept-Dec 05).**

Ram's project deals with the synthesis of process water systems that integrate the water reuse section for processes with the distributed water treatment section for a given number of pollutants. The initial objective is to find for given sets of processes and given treatment units the optimal configuration of the system that minimizes the use of freshwater, or more generally that minimizes the total cost. Ram has assumed for the processes units that they are either characterized by fixed contaminant loads, or by variable loads that obey mass exchange constraints in terms of concentrations. For the treatment units fixed recoveries are specified. In a current extension he is considering the case of multiscenario problems in order to handle uncertainties in the contaminant loads and recoveries in the treatment units.

Ram has developed a superstructure that involves for a given number of process units and treatment units all possible alternatives for interconnection of process and treatment units, and mixing and splitting of streams. The model corresponds to an NLP model with bilinearities in the mixers given by the product of flows times concentrations in ppm of the contaminants. Ram has developed a global optimization algorithm that relies on

combining spatial branch and bound search, with piecewise linear approximations inspired by the work of Lorena Bergamini. The motivation is that piecewise linearizations improve the quality of the lower bound, but they do it at the expense of introducing additional 0-1 variables. For this reason it is sensible to still use a spatial branch and bound search, but strengthened by piecewise linearizations for a fixed (modest) number of intervals. To also strengthen the quality of the lower bound, Ram has derived a valid cut that represents overall mass balances for each of the contaminants. The algorithm also relies on bound tightening and on branching only on the flows. The bisection rule is used for partitioning.

Ram has tested his method with several examples. In one problem involving 4 process units and 3 treatment units the NLP had 195 variables and 151 constraints. CONOPT either did not converge, or if it did, the best it found was 186.18 ton/hr. Our proposed method converged to the global optimum of 170.39 ton/hr (see Figure below), requiring only 10.3 secs solving the problem at the root node. BARON in contrast required 3490.5 seconds and 9656 nodes. Ram has also extended the model to general cost functions and selection of treatment units, which gives rise to an MINLP model due to 0-1 variables that are needed to model these units. For this case Ram has solved a problem involving 2 contaminants, 4 process units and two treatment units, each with the choice of two technologies. Also concave cost functions were used. The size of the MINLP was 4 0-1 variables, 178 continuous variables and 190 constraints. The proposed method required 1 node and 2.3 secs to find the global optimum ($619,205), while BARON required 37621nodes and 17541 secs. DICOPT converged in this case in a suboptimal solution ($ 665,827). Ram has completed a manuscript on this work which has been accepted for publication.



As a next step in his research, Ram has considered the extension of the above problem to the case when the water system must operate under multiple scenarios in which the loads in the units as well as the recoveries in the treatment units are uncertain, and therefore change in each scenario. This problem gives rise to a two-stage stochastic programming problem. The first stage costs include the investment cost for piping which depends on the maximum flowrate allowable in a pipe, and the design cost of each treatment unit, which is dependent on the maximum flow of wastewater handled by that treatment unit. The operating costs of the network appear in the second stage, which include the cost of obtaining freshwater for use in the process units, the cost of pumping a certain flow of water through the pipes and the operating costs in the treatment units.. The difficulty of the global optimization for the nonconvex multiscenario problem is that the corresponding NLP or MINLP becomes much larger. Furthermore, it becomes necessary to introduce 0-1 variables for the piping in order to control the potential complexity in the configurations for each period. Ram has developed an initial version of a branch and bound algorithm that relies on a Lagreangean decomposition scheme for the generation of tight lower bounds at each node, in which the original model is decomposed into single scenario sub-problems that are solved to global optimality and from which valid cuts are generated. These cuts are then added to the original problem that is convexified by constructing convex envelopes for the non-convex nonlinear terms leading to an MILP that is solved to predict a rigorous lower bound to the global optimum). A heuristic is used for the generation of good upper bounds. These lower and upper bounds are converged within a specified tolerance in a spatial branch and bound algorithm. Ram considered a problem with 2 process units and 2 treatment units and 10 scenarios. The MINLP model involved 28 binary variables, 868 continuous variables, 1044 constraints and 490 non-convex terms. The application of the proposed algorithm yields an expected cost of $651,653.06, which is the global solution to the problem. The lower and upper bounds converge within 1% tolerance at the root node of the branch and bound tree. The proposed

algorithm takes a total of 62.8 CPUsecs to solve while BARON could not verify optimality of the upper bound after 10 hours of CPU time.

Eugenio Bringas

The aim of the work by Eugenio, which was conducted in collaboration with Ramkumar, was to obtain the globally optimal design of an emulsion pertraction plant, that consists of a prespecified number of hollow fiber modules (MOD), mixers (MU) and splitters (SU), with various possible interconnections between the units. The specific objective of this work has been to identify the interconnections of the superstructure and the flowrates and the contaminant compositions of the streams, such that we meet the discharge composition regulations using a minimum area of the membranes. In order to address this problem, Eugenio proposed a superstructures for the aqueous feed solution and the emulsion stream which flow counter currently inside a hollow fiber module where the transfer of contaminant takes place between the aqueous phase and the emulsion phase. In the postulated structure, the aqueous phase flows continuously, while the emulsion phase operates in batch mode.

Eugenio initially modeled the problem in a rigorous way making use of differential and algebraic equations for the hollow fiber modules. The resulting NLP is, however, highly nonlinear and nonconvex which makes it very difficult to solve to global optimality. For this reason he simplified the model and solved this simplified model to global optimality. This globally optimal solution is used as a initialization for optimizing the rigorous model. The global optimization algorithm relies on a Lagrangean decomposition based spatial branch and bound algorithm in which tight lower bounds on the global optimum are generated. These lower bounds are made to converge to the solution in a branch and bound setting. The Lagrangean relaxation of is decomposed into two subproblems pertaining to the aqueous phase and to the stripping phase which are optimized independently for fixed values of the multipliers. Eugenio applied this technique to a system consisting of 4 membrane modules. To determine the optimum number of modules the easiest approach is to simply enumerate the different alternatives. Eugenio is completing this work in Spain, and completing a manuscript on it.

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: Optimization strategy for synthesizing heat integrated/thermally integrated columns

Collaborators: Jose Caballero [Associate Prof., Univ. Alicante]

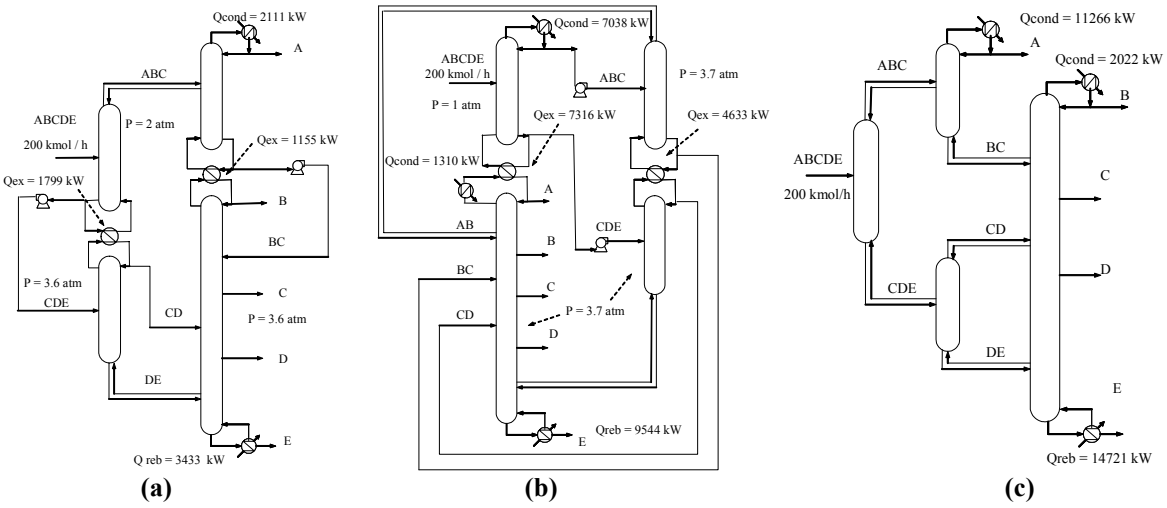
This project deals with a modeling framework for separation systems based on the State-Task Network (STN) and State Equipment Network (SEN) representations. These models are formulated with generalized disjunctive programming (GDP) models that explicitly handle discrete and continuous variables. The intent has been to develop whenever possible optimization approaches that can make use of tray by tray models. In the recent past Mariana Barttfeld from Argentina concentrated on MINLP and GDP models for single columns and complex column configurations. Currently Jose Caballero in Spain is working on the analysis and synthesis of thermally integrated columns using short-cut techniques for predicting the performance of the columns.

In the past Jose has addressed the issue of systematically generating all the configurations for thermally coupled distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. 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 developed a novel superstructure for synthesizing non-azeotropic mixtures with the Underwood-Fenske-Gilliland approximations. The synthesis approach considers alternatives from conventional sequences, in which each final distillation column has a condenser and a reboiler, to fully thermally coupled distillation sequences going through all possible intermediate combinations. In order to perform the optimization of the superstructure Jose formulated the problem as a disjunctive programming problem, and developed a two-stage solution procedure. In the first one a sequence of tasks is optimized, and then in a second stage the best configuration in actual columns is extracted among all the thermodynamically equivalent configurations. The model has proved to be robust and reliable. The more complex example involved 5 alcohols (ethanol, isopropanol, 1-propanol, isobutanol, 1-butanol). The optimal configuration

involved 5 columns with 24 trays (AB/BCDE), 45 trays (BCD/E), 40 trays (BC/D), 120 trays (A/B) and (B/C) 29 trays. The CPU-time required was several minutes. Rigorous simulations in HYSYS showed very good agreement with results presented.

In his recent work Jose has been investigating a strategy for determining optimal design of distillation columns using a process simulator (ASPEN) and using the disjunctive programming framework. A major motivation has been to avoid the need of explicitly handling the thermodynamic equations as has been the case in Mariana's work. The idea in Jose's model is to adopt the Logic-Based Outer-Approximation Method in which the NLP subproblem is given only by the existing trays in the column. For this Jose uses the optimization capability in ASPEN to optimize a column with fixed number of trays. In order to define the MILP master problem Jose performs numerical perturbations on the degrees of freedom (usually only two variables). In addition he performs a sequence of simulations by adding and deleting trays in each section in order to evaluate the economic potential of these decisions which are modeled as 0-1 variables in the MILP. This scheme has proved to be quite successful. So far largest problem that Jose applied it was to a mixture of 2-propanol, 1-propanol, i-butanol and 1-butanol. A column with 70 trays was postulated (feed in tray 35). The optimum was found in 3 major iterations. The design yielded a column with 27 trays (tray 24 to 57) and was solved in about 1 min CPU-time. Jose is finishing the testing of this method with few more examples. A manuscript has been written describing this work.

In the recent work of Jose he has dealt with the synthesis of mixed thermally coupled-heat integrated distillation sequences. The approach considers from conventional columns (each distillation column with a condenser and a reboiler) to fully thermally coupled systems (only one reboiler and one condenser in the entire system). Jose has considered the generation of the superstructure generation using a representation based on separation tasks instead of equipment. To derive all feasible structures, ranging from thermally coupled to simple columns, Jose has written the logic using propositions in Conjunctive Normal Form (CNF). Converting these propositions into Disjunctive Normal Form (DNF) yields each of the feasible design alternatives. The problem is that this transformation is non-trivial. However, Jose considered three possible approaches. One is to pose the CNF logic as a constrained logic programming problem. In this case by using OPL one can in fact generate all solutions to the CNF propositions that are equivalent to each of the clause in DNF form. The second approach is to convert the CNF logic into linear inequalities and pose the problem as an integer program with zero objective. In this case by using BARON one can find all the solutions to the integer program, which again represent each term in the DNF form. The reason this development is significant is that w have now a systematic way of generating the DNF logic for superstructures. The third approach is a recursive ad-hoc procedure on the graph of the superstructure that Jose implemented in MATLAB. A disjunctive programming formulation that incorporates the logic constraints was developed by Jose. The model is based on the Fenske, Underwood Gilliland equations. However, the disjunctive formulation allows easily the use of any other shortcut, aggregated or even rigorous model without almost modifying the structure of the formulation. Rather than solving the problem with a general purpose algorithm Jose has developed a specific solution method that consists first of solving the MINLP problem (big-M reformulation of GDP) with DICOPT assuming no heat integration. Fixing the sequence of states from the first MINLP, the heat integrated problem is solved with SBB. The algorithm then sets up an OA master problem from which the nest sequence of states is generated and iterated with the MINLP problem with fixed sequence of states. Jose has tested this algorithm in 3 examples ranging from (a) 5 hydrocarbons to (b) alcohols to (c) aromatics. The interesting feature in the examples is that the method generates structures with both thermal integration and heat integration, and only thermal integration as seen below. Jose has just completed a manuscript on this work which has been submitted for publication.



Synthesis of Crystallization Processes

New developments: **Integrated optimization for crystallization process with refrigeration system**

Post-doctoral fellow: **Carlos Mendez (started Janaury 2003)**

In a joint collaboration project with Jeff Logsdon, John Myers and Scott Roberts from BP, Carlos first addressed the separation of paraxylene, orthoxylene and methaxylene through a crystallization process given that their boiling points are very close making the use of distillation unattractive. Carlos developed an NLP optimization model for the operating and design optimization of a fixed configuration of a crystallization process for the separation for paraxylene. The process involves crystallizers, reslurry drums, centrifuges, heat exchangers and a refrigeration system. The model, which makes use of short-cut equations for predicting the mass and energy balances and sizes, and simply assign costs for refrigeration, is quite challenging to converge due to the nonlinearities involved. To circumvent this problem Carlos developed a two-stage procedure the increase the robustness of the convergence. The proposed model has been extended recently as an MINLP model for optimizing the topology of the flowsheet and as well as the operating conditions. The first step involved the optimization of the topology for the crystallizers. This has involved a superstructure that is similar in nature to the Floudas superstructure for heat exchanger networks, except that several exiting streams from the crystallizers that are directed to the others can be eliminated since each crystallizer does not maintain a unique identity as is the case of matches in heat exchanger networks. The results have shown that the predicted structure tends to have fewer crystallizers than the ones used in practice. More recently Carlos has been able to perform the optimization of the entire superstructure considering two and three stages of crystallizers and reslurry drums. The results have indicated that the three stage system may be advantageous since the recycle is significantly reduced for this case.

In order to explicitly include the refrigeration system as part of the optimization of the crystallization process, Carlos has considered a superstructure that is similar in spirit to the one we had developed many years ago in the Ph.D. work of Mark Shelton. At that time temperatures had to be discretized in order to reformulate the problem as an MILP. In this case Carlos was able to use continuous temperatures which gives rise to an MINLP problem. He has considered a cascaded refrigeration system consisting of two cycles (ethylene and propylene) where the number of stages are to be optimized. The model relies on a number of short-cut and empirical thermodynamic, efficiency and cost correlations that provide good agreement with real plant data. Carlos was able to successfully solve this model for fixed loads of the crystallization system.

In the final stage of this project Carlos considered the simultaneous optimization of the crystallization process with the refrigeration system. To avoid the solution of the entire MINLP in one single step, Carlos initializes using a sequential strategy. That is the crystallization process is first optimized using nominal costs for the refrigeration. Once the loads are determined the refrigeration is synthesized for these fixed loads. This design, which is a "typical" sequential design provides good initial values for the simultaneous MINLP problem. Carlos solved the problems for

a variety of acses (e.g. two and three stages, different equipment). He found that the integrated model led to modest savings in total cost, but that typically reduced energy costs (mostly electricity from refrigeration) at the expense of increased investment costs in the refrigeration system. Carlos will be putting together a short paper to summarize the findings of this work.

Optimization Approaches for Metabolic Engineering

New developments: **Selection of screening strategies for NMR analytes with Analytical Hierarchical Process**

Student: **Soumitra Ghosh (Ph.D., started Jan 02) (supervised jointly with Mike Domach)**

This project on metabolic engineering by Soumitra Ghosh is in collaboration with Mike Domach. The first part of Soumitra's work involved the development of a software package for systematically identifying all the alternate optima that arises in the LP problem for maximizing yield in metabolic networks. The methods he implemented were a recursive MILP method that was developed by Sangbum Lee and a depth-first enumeration method. These methods can provide information on product yield horizons and the optimal "target" values of fluxes to achieve in metabolic networks. These methods can also elucidate the metabolite trafficking possibilities in tissues. While methods that enumerate flux scenarios are useful for the "front-end" analysis of metabolic engineering problems or probing the possibilities in tissue physiology, the evaluation of actual data from a tissue or engineered cells is ultimately needed to verify the veracity of theoretical predictions and mechanistic hypotheses. This gives rise to an inverse problem in which NMR data are used to best fit a linear combination of fluxes that minimizes a sum of squares deviation. However, this nonlinear programming problem is problematic because it is highly non-convex due to the bi-linear and tri-linear terms that arise in the isotopomer distribution vectors. Therefore, in order to obtain reliable results, it is imperative to solve the NLP to global optimality. For this purpose Soumitra has developed a formulation that involves using the results of the "front-end" analysis (MILP solutions) to provide tight bounds in the global optimization of the inverse-problem of data-to-fluxes. Soumitra has applied the code BARON by Nick Sahinidis for deterministic global optimization and obtained good results. He first applied it in a small hypothetical problem in which BARON only required 2.3 seconds to find the global optimum. The problem involved 51 variables and 47 constraints. He then considered an E. coli bacterial mutant that has had pyruvate kinase activity deleted with 17 reversible reactions. The problem involved 910 variables and 897 constraints, and was solved by BARON in about 3 hours. It should also be noted that linking flux distribution forecasting with spectra-to-fluxes calculations provides a potential means for assessing the utility of different analyte sets for ascertaining the net values of metabolic fluxes. Such linked tools may assist in forecasting physiological possibilities in metabolic engineering and in tissue studies as well as help with closing the loop between physiological reality and the system "model" the investigator has conceived.

Soumitra has recently developed a two-tiered computational approach for screening NMR analyte sets for their ability to report on metabolic fluxes. After obtaining the flux bounds via MILP, analytes are first screened for the ability of their NMR spectra to differentiate between different extreme point (or linear combinations of extreme point) flux solutions. Then, the analytes are screened for whether they provide unique flux values or multiple flux solutions – this is achieved via determination of possible multiple global solutions of the inverse optimization problem. The effect of noise in NMR data is also being considered as a factor in the ability of an analyte set to faithfully provide a correct flux solution as opposed to an alternative solution. The screening strategies have been successfully implemented in a small hypothetical problem and in the E. coli system. An additional aspect that Soumitra has considered is the sensitivity problem of the inferred metabolic pathway with noise measurements in the NMR spectra. His has formulated this problem as an NLP problem to determine the maximum of the minimum deviations in the different peaks of the spectra given that the pathway fluxes lie within a given tolerance. With this additional measure and economic considerations of analyte selection that is driven by the material and labor costs associated with their isolation, there are different trade-offs that one can consider in the selection of the analytes. In order to address this problem Soumitra has applied the Analytic Hierarchy Process or AHP by Saaty. In simple terms the AHP leads from simple pairwise comparison judgments to the priorities in the hierarchy. Soumitra considered the performance of each NMR analyte according to the following criteria: (i) extreme point comparison (ii) abundance data based on both cytosolic content and frequency in proteins , (iii) Multiple Global Optima Test. Glutamate ranked first overall, followed by Alanine, and OAA (aspartate). This ranking was consistent with the

results of the structured methodology used in this work. Soumitra is currently completing a manuscript on this work for which he has described the AHP procedure in an algorithmic fashion.

Multistage Stochastic Optimization for Design and Planning of Oilfield Infrastructures

New Developments: **Pending publication of two papers.**

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

Vikas completed his Ph.D. degree and joined the Upstream Research Center of ExxonMobil in Houston last August. The specific problem that Vikas has considered in his project 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, whereas the rest are uncertain and described by discrete probability distribution functions. 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 developed a multistage stochastic optimization in which the investment decisions define the structure of the scenario tree. Vikas also generalized the problem for general purpose linear multistage stochastic programming..

Vikas first discovered the interesting point in the gasfield problem that given uncertainties in the size and deliverability, the tree of scenarios is dependent of when the investment decisions are made. Based on this observation, Vikas formulated the variable scenario tree/multistage optimization problem 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 first 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 (wait and see). Next, at each 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 solved in order to yield a lower bound. Since this multistage problem can become very large, Vikas used a shrinking horizon approach to avoid the simultaneous solution in the full space. The procedure is continued until the lower and upper bounds lie within a given finite tolerance. The largest problem that Vikas solved involved 4 certain and 2 uncertain fields in 8 years. The number of scenarios was 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 and had an expected NPV of $79 million, a $5.6 million improvement over a deterministic solution.

Motivated by Vikas' work in the multistage stochastic optimization of gasfield problem, he generalized the scenario decision dependent problem to general linear stochastic programming problems. The interesting contribution by Vikas was that he was able to develop a closed-form disjunctive programming formulation in which the variable structure of tree is handled through disjunctions. This was accomplished by first representing the stochastic problem through disaggregated states at each time period. These are enforced to be the same through "non-anticipative constraints" that ensure that the states be the same when the endogenuous uncertainties are not revealed because no decisions are made. Otherwise, they "explode" into the nodes that define the events in the tree. The drawback of this model is that the number of disjunctions is very large since all possible pairs of discrete-states defined by discrete probabilities must be considered. To reduce the size of the problem Vikas showed that it is sufficient to consider only successive adjacent pairs which significantly reduce the size of the problem. For larger problems, however, the reduction is insufficient. To circumvent this problem Vikas developed a branch and cut method in which the disjunctions are dualized so that the nodes involve a Lagrangean relaxation subproblem which yields stronger lower bounds than the full space 0-1 relaxation. Furthermore, the bounds can also be strengthened with a lot-sizing reformulation. For the application of the Lagrangean based branch and bound method he considered a manufacturing problem that has been addressed by Jonsbraten ("sizes problem"). The problem is similar to a lot-sizing problem but also involves manufacturing parts in different sizes. When Vikas' solution method was applied to the largest problem it involved 3,136 0-1 variables, 60,993 continuous variables and 181,939 constraints! This very large problem was solved with the proposed method within 0.038% of optimality in only 3 nodes requiring 13,507 secs (about 3 hours 45 minutes). In contrast, a conventional LP-based branch and bound solved the problem in about 37 hours within 0.3% of optimality and requiring 71,151 nodes. The manuscript describing this work has been submitted and is in press in the journal *Mathematical Programming*.

In the last part of his Ph.D. thesis Vikas developed in collaboration with Amr El-Bakry and Eric Mulkayan from ExxonMobil an implementation in C++ of the branch and cut method described above for solving stochastic programs with decision trees that are dependent of design decisions. The goal of this implementation is to have a general computational tool that can be more easily adapted to the solution of a variety of stochastic problems. In this method non-anticipativity constraints are dualized while disjunctions are relaxed. In this way nodes involve a Lagrangean relaxation subproblem that involves the solution of MILP subproblems for each scenario. The advantage of the approach is that it yields stronger lower bounds than the full space 0-1 relaxation. Vikas developed the C++ implementation using an object-oriented modular framework. Major modules include preprocessing, bounding, branching, feasibility generation, and were interfaced with CPLEX. Vikas applied his method to gas field problems that ranged from 3 to 81 scenarios per time period, which in turn gave rise to MILP problems that involved from 594 0-1, 4480 continuous and 7457 constraints to 16,281 0-1, 125,956 continuous and 386,597 constraints. These problems were solved in 169 secs for the smallest and in 37,204 secs (over 10 hours) for the largest. Vikas compared the performance with a direct solution of the MILP using CPLEX. By allowing 10 times the CPU time for Lagrangean relaxation, CPLEX was faster in the smallest problem (49 secs), but in all others it did not terminate in in same cases obtained a solution that was significantly lower in profit (e.g. 71 vs 86). Vikas has produced a manuscript on this work which has been submitted for publication.

Strategies for Reduction of Time-Varying Uncertainty in the Planning of Process Networks

New Developments: **Disjunctive/MILP model**

Students: **Bora Tarhan (Ph.D. started January 2005)**
Visitor: **Sergio Frausto (Inst. Tecnologico Celaya, July-Dec 2005).**

Bora Tarhan, a new Ph.D. student who will follow Vikas' line of work, has been addressing the following stochastic optimization problem. A network of candidate processes is given over a specified time horizon that is described by multiple time periods in which product demands are specified. It is assumed that major uncertainties are involved in the yields of each process, which are described by probability distribution functions. We consider that the uncertainty can be reduced with the potential investment in pilot plants, which delays the introduction of a process but provides more accurate process information on the yields. In addition, it is assumed that once a process is installed, the uncertainties in the yields decrease with time to reflect the experience and improved understanding in the operation of the process. The problem then consists in making planning decisions for process selection, capacity expansions, and possible investment in pilot plants in order to maximize the expected net present value over the specified time horizon.

In order to capture all the complex trade-offs, Bora has developed a new mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints that are similar in spirit to Vkas's model. However, one importance difference is the time varying uncertainty. For simplicity Bora considered that this uncertainty is revealed over two time periods. Furthermore, he assumed that the time required for a pilot plant study corresponds to one time period, meaning that it reduces the uncertainty to only one time period. Obviously this scheme is rather restrictive but we have adopted it only as an initial assumption that we intend to relax at a later stage. In order to solve this special multi-stage stochastic program he has reformulated it as a mixed-integer linear program, which can be solved through an LP-based branch and bound for smaller instances but that leads to a very large problem. Therefore, Bora has proposed a solution strategy that relies on the successive calculation of lower and upper bounds of the expected net present value. The basic idea for finding upper bounds is to reformulate the multi-stage model having time varying gradual uncertainty resolution as smaller problems having immediate resolution. Combining the decisions from smaller problems yields a feasible solution which is a lower bound for the model. Upper bounds are generated using Lagrangean relaxation. The corresponding subproblems are obtained by relaxing the disjunctions and adding the first period non-anticipativity constraints to the objective function with Lagrange multipliers. The resulting model can be rewritten as independent subproblems for each scenario. The overall objective is to find the minimum upper bound by updating the multiplier. This scheme can be extended as a branch and bound method to reduce the gap, but that will be considered in future work. Bora has successfully applied this method to a small 3 process network, with one existing process and two with new technologies and for which investment of pilot plants can be considered. A 10 year horizon was considered. The problem was solved within 2% tolerance of the upper and lower bounds with the proposed method. The solution proposes expanding

Process I up to a capacity of 10 tons/day and making an additional expansion of 4.93 tons/day at time period 3 if the yield turns out to be 69%. If the yield for Process I is found to be 81% then an expansion of 2.98 tons/day is made at the time period 4. This solution that does not involve the use of a pilot plant, yields an expected net present value of $8,050,500.

Sergio Frausto

Sergio considered the design of process networks with uncertainties in the demands. He formulated the problem as a two-stage programming problem with continuous distributions. Rathyer than discretizing these distributions he applied a stochastic decomposition methods that relies on sampling using Hammersly sequence. The idea is to generate a sample of a given number of points. The problem is then solved sequentially with the L-shaped method (i.e. through its dual). The results showed that in fact there was not much of a difference when discrete distributions are used. This reflects a result that has been known in the "folklore" of stochastic programming, namely, that results in terms of decisions (not objective function) are not that dependent on the "uncertainty" of the distributions. A qualitative explanation of this is that the multiscenario optimization has the effect of smoothening the effect of the decisions.

Simultaneous Planning and Scheduling of Continuous Multiproduct Plants

New developments: Development of aggregate and detailed models

Students: Muge Erdirik [Ph.D. started Jan 2004]

Muge's project deals with the simultaneous planning and scheduling of continuous multiproduct plants. The initial objective in her work has been to consider the case of a single processor on which a number of products must be produced over a given number of time periods. Sequence-dependent changeovers are given and due dates are assumed to take place at the end of each time period. The objective is to determine a production plan and schedule in order to maximize the profit (income minus inventories and changeovers).

To address the scheduling problem described above, Muge has first developed a detailed MILP scheduling model using the concept of slots. This model, while accurate, can only solve problems with few time periods, meaning it cannot be used to solve planning problems that typically require long time horizons. A simple approach to circumvent this problem is to develop an aggregate planning model that is simpler to solve but does not include all details such as changeovers. Well-known limitations of such an approach are inconsistencies between planning and scheduling and loss of optimality. Therefore, our objective has been to develop an iterative scheme that relies on aggregated models but that is guaranteed to converge to the same solution as if we had solved the detailed scheduling model. In order to accomplish this objective Muge developed an aggregated MILP model that underestimates the changeover times and includes 0-1 variables for deciding what products may be produced in a detailed schedule. The iterative scheme consists in solving a sequence of aggregated MILP planning models and detailed scheduling models with fixed assignment of products to be produced at each time period. In addition to using a simple integer cut, Muge has developed superset, subset and capacity cuts that eliminate a larger number of alternatives. The idea of the supercuts is to eliminate those alternatives that involve a larger number of products that the current assignment. These can be eliminated on the basis of optimality arguments. Likewise the idea of subset cuts is to eliminate subsets of alternatives from the current assignment. These are eliminated on the basis that subsets are considered in the detailed scheduling level since the 1-assignments are treated as upper bounds; only the 0 assignments are fixed. The capacity cuts take into account the potential effect of changeovers in limiting the production. For the cases where the detailed scheduling model with fixed assignments can still be expensive to solve, we can resort to a rolling horizon solution approach or on a temporal decomposition scheme.

Muge has tested extensively her solution method. She considered two major cases: high lower bounds for the demands bound, low lower bounds for the demands. In the former case the schedule is forced to produce more products in each time period, and hence is more difficult to solve. She considered 5 products and a time horizon ranging from 4 to 24 weeks. The trends in the results were as follows. In the 4 week problem (120 0-1, 987 continuous, 906 constraints) the proposed method converged to the optimum in 207 secs while the detailed model over the 4 weeks did not terminate the search after 6000 secs (8% gap of bounds) and obtained a suboptimal

solution. In the case of low demand the proposed method converged in 4.6 secs versus 525 secs for the simultaneous approach. In the 24 week problem (720 0-1, 5907 continuous, 5526 constraints) the proposed method converged within 6% of the optimum in 3190 secs while the detailed model did not terminate the search after 4000 secs (18% gap of bounds) and obtained an inferior solution. In the case of low demand the proposed method converged in 8 secs within 4% of the optimum while the simultaneous approach did not terminate after 3000 secs but found a slightly better solution. Muge has completed a manuscript on this project which has been accepted for publication.

Over the summer Muge spent an internship at Dow Chemical in Midland where she has addressed a simultaneous multisite planning and scheduling problem for batch reactors. This problem is in fact the case study that was selected by Dow for the Enterprise-wide Optimization project. The specific problem can be stated as follows. It is assumed that we are given a set of production sites, each with a unique set of raw material costs, raw material availability, storage tanks with associated capacity, transportation costs to each customer, reactors with associated materials it can produce and batch sizes and times for each material it can produce, as well as operating costs for each material, sequence dependent clean out times, and time the reactor is available during a given month. We are also given a set of customers, each with a unique set of demand for desired products, and price paid for each product. Finally, specified are the materials produced: process intermediates and final products. A related issue is the assignment of the limited number storage tanks at a site to particular materials. Generally a tank can store any material produced at a site, but due to the costs associated with setting up an inventory tank for a particular material a tank cannot be arbitrarily switched between products month to month but must be assigned a product for at least 6 months. Another issue is that a final product of one process may be used as a raw material for another process within the site. However, once a final product is fed to the dedicated storage tank, it can not be retrieved back to the plant. Therefore, one has to take into account the issue of intermediate storage as well. The problem is then to determine the monthly production quantities for each reactor and the assignment of materials to storage tanks such that the profit is maximized.

In order to tackle the above problem Muge intends to develop for the entire system of sites and customers a similar bilevel decomposition as the one for the continuous single-stage problem. The major difference, however, will be that instead of having a continuous single stage plant we will have multiple sites each consisting of a two stage batch process with parallel reactors and storage tanks. The bilevel temporal decomposition for this multisite problem can lead to potentially very large MILP problems for both the upper and the lower levels. Therefore, we plan to investigate the decomposition of these problems through a temporal Lagrangean scheme (similar to our previous work with Jennifer Jackson). That is, at the solution of each upper and lower level problem we would decompose the corresponding multisite problem by dualizing the inventory constraints, so that the subproblems in the Lagrangean decomposition can be solved independently for each time period. For the aggregated planning model Muge has developed a model that represents a relaxation of the STN model and in which time balances are performed for each unit and integrality is imposed on the number of batches. This model was applied to a problem consisting of 4 raw materials, 6 products and 2 reactors over a 4 week period. The proposed model predicted a profit of $1,134,000 while the detailed schedule that was obtained with the RTN model predicted a profit of $1,032,000. The aggregated MILP model only required 10 CPU secs while the detailed MILP scheduling model required 2360 secs. For the scheduling part Muge is currently exploring a slot-based model in order to properly handle the sequence dependent changeovers.

Cost Models for Contracts in Supply Chain Optimization Problems

New Development: **Disjunctive cost models for a variety of contacts yield effective MILP models**

Visitors: **Minhwan Park (KAIST)**
Fernbando Melle (Polytecnic University of Barcelona)

Minhwan and later Fernando, addressed the issue of modeling contracts in supply chain optimization problems motivated by the fact that conventional models usually simply assume fixed prices of the raw materials and products. They considered short and long-term multiperiod production planning of a chemical supply chain network over a given number of time periods. The operation of the network is constrained by existing capacities of all processes in the network, limits in the supplies of raw materials and market saturation of some products. Information is given for different types of contracts that can be made for purchasing raw materials and selling the products. The

objective in the short-term planning problem is to determine over a given time horizon, typically weeks or months, the types of contracts for the purchase of raw materials and sales of products in order to maximize the profit, which can be calculated by the data on sales revenues, operating costs, marketing costs, inventory cost and shortfall penalties. For the case of the long-term planning problem, the possible capacity expansion of the processes is considered. In this case, the NPV is optimized. The goal in these problems is to decide (a) which contract to make in the purchase of the raw materials and selling the products in each time period, and (b) whether capacity of each process should be expanded or not in each time period.

Minhwan and Fernando considered the following supply/demand models: fixed price contract, discount contract, bulk discount contract and fixed duration contracts over a specified number of time periods. For each of these contracts disjunctive programming models were proposed which in turn were formulated as MILP models using the convex hull reformulation. These contract models were then incorporated in the corresponding multiperiod MILP models for short and long term planning. These models were applied to a petrochemical complex involving 28 chemicals and 38 processes. Both short term (10 months) and long term (4 years) problems were considered. For the first case when only fixed prices are considered the planning problem reduces to an LP with 12,606 continuous variables and 13,416 constraints. When the four types of contracts are considered for 3 of the raw materials (naphtha, ethylene and acetylene) this gives rise to an MILP with 6160 0-1 variables, 40,606 continuous variables and 46,002 constraints. To our surprise CPLEX took only 0.995 sec to solve this MILP (vs. 0.18 for LP). The explanation is that the disjunctive models are extremely effective and provide very strong LP relaxations. In the long term problem we observed a similar trend. The case of fixed prices involves 152 0-1 variables, 5161 continuous variables and 5269 constraints, while the case of contracts also on the same raw materials involves 2,616 0-1 variables, 12,329 continuous variables and 14,017 constraints. In this case CPLEX actually took less to solve the problem with contracts (0.89 sec vs. 1.2 secs). The results also show qualitatively the advantages of the flexibilitry provided by the selection of contracts, both in terms of increased profits and in terms of demand satisfaction. A paper describing this work has been completed and is available to CAPD members.

Scheduling of Batch Multiproduct Plants

New Development: **Computational strategies for large scale industrial problem**

Post-doctoral fellows: **Carlos Mendez (started Janaury 2003)**
Pedro Castro (finished July 2005)

Carlos Mendez

In collaboration with Iiro Harjunkoski and Marco Fahl from ABB, and from Jaime Cerda at INTEC, Carlos has completed a comprehensive review of the area of batch scheduling. In this paper a general a roadmap is given for classifying the problems as well as the optimization models. The models are then reviewed according to the classification with their main equations from the standpoint of discrete and continuous time STN and RTN models, and from the standpoint of sequential models for multistage plants. Numerical results are presented for discrete and continuous time models for a well-known Kondili example and an industrial size problem proposed by Kallrath from BASF. These results were obtained by our visitors from Barcelona, Anna Bonfill and Gonzalo Guillen. The paper next discusses a series of real world examples to illustrate the considerations that future methods must account for. The paper then reviews academic and industrial research with reference to commercial software. Finally, the paper discusses other solution approaches, the need to use special strategies for large industrial problems, and the area of rescheduling. We believe that it should be very useful for those who want to get acquainted with the batch scheduling area. The manuscript has been submitted for publication and is currently being revised by us.

Pedro Castro

Pedro Castro has returned to INETI in Portugal. He made important contributions with a continuous RTN model (Resource Task Network) in his Ph.D. in Portugal, and used it as a theme for his research at Carnegie Mellon. In the RTN is the model is viewed as a balance of resources (of equipment, states, utilities, manpower, etc.). Pedro first examined the single stage problem with parallel lines, a problem that Vipul Jain addressed in his Ph.D. thesis. Pedro also found like Vipul Jain that the MILP and CLP models increases exponentially with problem size, while the

hybrid MILP-CP method attains reductions of several orders of magnitude in the larger instances. He then also found that his continuous time RTN model exhibits exponential behavior. However, he found if that he does not use a common time grid for the parallel stages, but that rather uses a multiple time grids for each stage, then the RTN MILP model can be solved almost as fast as the hybrid model. He solved problems ranging from 12 orders and 3 units, up to 30 orders and 5 units for the cost minimization case. This was a truly a surprising result because it comes to show again the impact that alternative formulations can have in solving MILP problems. Another interesting result that emerged was that Pedro solved the discrete time model with up to about 400 time intervals in order to obtain exact or very close approximations. The surprising point here was that while the discrete time model was slower for the smaller problems, it did not experience an exponential increase in time. In fact the times ranged from 2.5 to 27 seconds for all the test problems. Pedro also examined the performance when the objective is minimization of earliness. In this case the discrete model performed the best followed by constraint programming. This comes to show the importance of objective functions in scheduling problems. This paper has been accepted for publication and is under revision.

In the next phase Pedro investigated the optimal scheduling of multistage plants. In this case he performed a non-trivial extension of the multi-time grid RTN MILP model for a single stage. He also examined in detailed a sequential MILP model that had been proposed previously by Harjunkoski and Grossmann. He performed extensive numerical experiments using as objective functions cost minimization, minimization of makespan, and earliness minimization. The problems ranged from 6 orders, 4 units, 2 stages to 10 orders, 8 units, 4 stages. His results showed that constrained programming tended to be the more effective solution method for makespan minimization. The sequential model proved to be best for earliness minimization, while the proposed model performed best for the cost minimization criterion. On an overall basis, the discrete RTN model was also competitive. Here again the discrete-time formulation was shown to have very good performance, particularly for total earliness minimization, despite generating very large MILPs when considering the exact problem data. The trend that was also observed is that continuous time models were more effective in small to medium size, while discrete time was better for the larger problems. The main conclusion was that for the multistage case not a single model proved to be the dominant one. This work also led to a manuscript that has been accepted for publication.

Finally, Pedro was also involved in a challenging industrial pharmaceutical problem that was supplied to us by ABB through Iiro Harjunkoski and Marco Fahl. This problem had the feature that it is multistage, but with very significant changeover times, and with complex operating rules. Both, 30 and 50 order problems proved to be unsolvable with known existing MILP methods. Pedro and Carlos proposed two alternative heuristic decomposition approaches for the efficient and fast solution of large industrial scheduling problems. Both use the concept of decomposing the full problem into several subproblems, each featuring a subset of the orders. The main difference lies in linking the consecutive subproblems. While the first approach completely freezes the schedule of the pre-assigned orders and ensures feasibility for the remaining through machine release dates, the second approach allows for more flexibility by only fixing the assignments and relative positions of the previously scheduled orders. The second approach was found to be more robust and seems better suited for the solution of this specific type of problem. Using both approaches Pedro and Carlos were able to obtain solutions that are often very close to the global optimum. The results for the solution of a 30-order problem show that the proposed decomposition methods are able to obtain solutions that are 35% better than those obtained by the solution of the full problem, on a fraction of the computational time. The manuscript describing this work has been completed and is available.

Optimal Scheduling of Refinery Operations

New development: **Sufficient condition for converegence**
Postdoctoral fellow: **Carlos Mendez (started Jan 2003)**

Carlos worked on a joint collaboration project with Iiro Harjunkoski and Pousga.Kabore from ABB in the area of scheduling of petroleum refinery operations. The major goal was to develop a multiperiod model for optimizing the production planning and blending operations in a refinery. The specific problem is to consider a set of product demands over a specified time period for which one has to determine what intermediate products should be allocated to what blender at what time period. Carlos developed a novel recursive LP model for blending that is based on the idea of formulating volumetric and gravimetric properties with linear constraints, while computing the mismatch of

the nonlinear properties with linear approximations, from which a correction factor is inferred for the LP model. This correction is applied recursively, and convergence to good solutions is typically very fast (e.g. 3 iterations). This LP model is then incorporated as part of the MILP scheduling problem where decisions are made for the allocation of blenders and tanks, timing of operations, and amounts of products to be produced and their quality for the given specifications. Carlos developed both discrete and continuous time MILP scheduling models. In this way, extending the solution method for blending, the simultaneous scheduling and blending problem is optimized by recursively solving either of the two MILP scheduling models that incorporate the linear approximations for the blending equations.

The proposed method has been tested with several gasoline mixtures involving 9 components and 12 properties (4 of them nonlinear). The proposed method yields approximations that are very close to the nonlinear model. For problems involving 8 days of operation, 3 blend headers, 12 storage tanks and 3 final products, the proposed method was able to predict solutions with significant improvements in the profit compared to sequential procedures where the blending and scheduling problem are decoupled. The computational cost of the recursive MILP is very small (under 1 minute of computation). The manuscript of this work has been submitted and is currently under revision. An important issue has been the theoretical justification for the convergence, as well as numerical comparison with NLP and MINLP solvers. We have developed a sufficient condition for the convergence of the proposed MILP method. Qualitatively the proof relies either on assuming that all nonlinear specifications are inactive in which case the MILP model is exact, or when they are active that the nonlinear properties are a weak function of the compositions, which ensures that the Karush-Kuhn-Tucker conditions are identical to the nonlinear model. However, in the latter case a global solution cannot be guaranteed. The manuscript has been accepted for publication.

Simultaneous Scheduling and Control

New development: **MINLP model for cyclic scheduling of multiproduct CSTR reactor**

Collaborator: **Antonio Flores-Tlahuacac (Professor U. Iberoamericana)**

This is a collaboration with Antonio Flores from the Universidad Iberomericana (Ignacio's alma mater). Antonio, being a control person, has been motivated by the idea of using dynamic models for control in scheduling problems. Given our interest in the area of scheduling, we decided to join forces in a work in which the basic idea is to combine a scheduling optimization model, with a dynamic model for the optimization and control of the transitions. In this work we have addressed the simultaneous scheduling and control problems for a continuous stirred tank reactor (CSTR) that produces multiple products within a cyclic schedule that involves sequence dependent transitions. We formulated the problem as an optimization problem. Integer variables are used to determine the production sequence and continuous variables take into account production times, cycle time and inventories. The scheduling part of the model is similar to our previous work with Jose Pinto. Because, dynamic profiles of both manipulated and controlled variables are also decision variables, the dynamic part of the model is formulated with DAEs. The resulting problem can then be cast as a Mixed-Integer Dynamic Optimization (MIDO) problem in which the objective function includes income from sales of products, inventory costs and transition costs that takes into account through quadratic deviation terms, the amount of off-specification material produced during product transition. To solve the MIDO problem the MIDO problem is transformed into an MINLP using orthogonal collocation, where initial guesses on the duration of the transitions must be provided. These are then revised in a subsequent optimization. Because of the highly nonlinear behavior embedded in chemical process models, the resulting MIDO formulation gives rise to an MINLP problem featuring hard nonlinearities such as multiple steady-states, parametric sensitivity, bifurcation and even chaotic dynamics.

Antonio has tested the proposed model on several example problems. In one the problem consists of scheduling 5 products, each of them having 3rd order kinetics in the CSTR, the predicted cycle time was 127 hours using a sequence B $\rightarrow$ A $\rightarrow$ E $\rightarrow$ C $\rightarrow$ D, in which the dynamics of the transitions was explicitly accounted for with . It should be noted that the solution of the resulting MINLP was quite difficult to converge, but was accomplished by generating good initial guesses from the dynamic simulation.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: Gabriela Garcia (started March 2000)

Gabriela Garcia has developed web interfaces that are available in:
http://newton.cheme.cmu.edu/interfaces

The current list of programs that we have available, most of them in our website, are the following:
(description in http://egon.cheme.cmu.edu)

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:

STN	State-Task-Network MILP formulation for scheduling multipurpose batch plants. Both the the Kondili, Pantelides and Sargent (1993) model and the Maravelias and Grossmann (2003) are implemented.
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) MILP for resource scheduling in new product development (Jain, Maravelias)

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 MILP for supply chain optimization of multisite facilities with flexible processes, intermittent deliveries, changeovers and inventories (Bok/Iyer)

Steinar Hauan's Group

Agent Systems in Engineering Design and Optimization

Students: John Siirola (PhD, completed May 2005), and Israel Owusu (PhD, started Jan 2004).

BACKGROUND

The main idea behind agent systems is to enable the study of large-scale engineering and design 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

The underlying approach asserts that our computing capabilities will increase significantly over the next decade and that the computational resources will be available in the form of distributed computer clusters. We believe this will change our perception of "effective computing strategies": instead of creating algorithms that reach a result in the minimum number of algorithmic steps, it will become more important to be able to use the available -- but distributed --computing resources in an efficient manner. This represents a shift in thinking from cpu time to wall clock time.

A key feature in our approach is the use of an agent-based architecture. In these systems many computational agents – or individually executing algorithms -- 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?

With the completion of John Siirola's thesis, the fundamental implementation of the agent system and its control structure has been established. We have completed preliminary studies of multiobjective optimization for NLP, MIP and (simple) MINLP systems and demonstrated the conditions under which the agent system performs well compared to traditional approaches. We have also established the concept of "Polymorphic Optimization" wherein the agent system simultaneously consider more than one mathematical model of our physical system that each (de)emphasizes a particular aspect of the model.

PROGRESS

From his initial studies in modeling of distributed systems, Israel has moved on toward distributed optimization of multi-unit supply chains. The initial approach has been to model large scale enterprise as an aggregate system composed of subsystems that are iteratively solved in isolation while exchanging information about their production levels, cost and unsatisfied demands. In a sense, this borrows from the idea of spatial decomposition except that -- at the topmost level -- we do not commit to a single approach for defining the subproblem objective functions but rather let these evolve over time. One obvious consequence is the loss of convergence properties -- or guaranteed global results -- but the gain is computational speed and thus ability to solve much larger problems to a good solution.

The approach has been implemented and tested on a multiproduct batch plant; each capable of producing a mixture of 3 different final products through a fairly complicated series of coupled intermediates. In contrast to previously published work in this area, the overall set of product demands is sought to be satisfied by a collection of up to 10

different plants; each of which have their own cost structure and (moderately) different processing time for each of the many intermediate steps needed for each final product. The goal is to achieve -- for the collection of plants as a whole -- a close to cost optimal solution with a minimum of unsatisfied demand.

Simultaneous solutions to the problem are possible, although they quickly become intractable due to the number of variables and the exponential performance of typical MILP algorithms. Instead, we introduce a number of policies that partitions the overall set of product demands between each plant and then solves the scheduling problem in each (sub)plant -- now small enough in size not to be affected by exponential solution times -- to local optimality.

The simplest scheme for partitioning the overall demands is to assign equal fractional demands to each subplant based on an estimate of their overall capacity. While straight forward to implement and use, it is unlikely to give particularly good results for an inhomogeneous set of plants. Instead, we iteratively use the marginal information obtained from the solution to the (N-1)th set of scheduling subproblems to generate the demand distribution for the (N)th iteration.

While this on the surface may appear to substantially increase the overall computational effort, all the subproblems are solved simultaneously on a dedicated computer node in our cluster. Preliminary results indicate that we can solve moderately sized problems to near optimality with substantial reduction in overall solution time. Furthermore, our formulation is nearly independent of the number of individual plants in the problem as the runtime of the demand allocation module is insignificant compared to the runtime of each of the subproblems being considered.

A number of demand partitioning strategies are being pursued. On a medium-horizon timeframe, we also intend to use the modeling framework being developed in Prof Ydstie's group to better define the boundaries and interactions between each subsystem in a way consistent with the theory of passivity-based control.

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 (PhD, started Jun 2003)

Collaborators: Tamal Mukherjee (ECE), Jim Hoburg (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 two types of customized microfluidic devices: (a) integrated system wherein multiple microfluidic components are combined to form a complete single-function analysis system, and, (b) multiplexing systems where independent subsystems are combined physically on the same structure to provide parallel and/or redundant measurements.

The core idea of this work is to reduce the design and verification time for custom-designs from months and years to days and hours by use of component models and software tools for simultaneous performance optimization, layout and routing of the individual chips in question.

PROGRESS

The main achievement in the Fall semester has been the creation of a system-level simulator capable of evaluating the performance of integrated Lab-on-a-Chip systems, i.e. an arbitrary collection of mixing, reaction, separation and injection unit operations. The simulator is capable of handling both steady state and transient units and defines a set of interfaces that makes it straight forward to add more new unit operations as they become available.

The underlying logic behind the simulator has 5 steps:

1) Build the LoC topology, i.e. the connections between each individual unit operation.
2) Automatically construct a Directed Acyclic Graph (DAG) of the topology and identifying the order in which the calculations should proceed.
3) Convert the DAG into an equivalent electrical circuit, i.e. a resistor network.
4) For each uniquely identifiable transient or steady-state phase in the overall system, solve the resistor network to obtain the (static) set of driving forces present in each unit, i.e. currents and voltages at each node in the network. The identification of system phases is done automatically based on analysis of the individual unit operations.
5) For each unit in the DAG, invoke the reduced order physical models in the proper order to solve for the flowing input-output systems in each transient stage of the overall simulation.

The system is implemented in C++ and designed to interface directly with standard circuit algorithms for VLSI design, i.e. approached to physical layout, block packing and circuit routing.

(b) A MEMS-based Gravimetric Biosensor

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

Collaborators: Todd Pryzbycien (Biomedical Engineering), Anna Liao (ECE) and Gary Fedder (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

So far all test of mechanical and electrical components are positive and we're starting to get a good handle on how to consistently process the chips in the cleanroom and wirebond the connections to enable mounting in ceramic packaging. Most of the work has been spent in the ECE MEMS lab using their optical equipment to detect mesh vibrations and from those, reliably estimate the physical properties of the chip. We also had to design and build 2 high-gain amplifiers to ensure we were able to detect the signals for higher order vibrational modes; a key step in the path toward the design of integrated arrays. We can now reproducibly detect resonance for various types of on-chip mechanical structures; this is verified both by a power spectrum as well as phase-angle measurements. In fact, the methods by which we now detect resonance are so sensitive that we reproducible detect differences between membrane types designed with different mesh structures, i.e. with different void fractions and thus weight.

In December, we obtained temporary access to a new generation optical probestation [$400k] that enables us to detect out-of-plane motion down to a few picometer range as well as focus on a (small) piece of the vibrating surface. This equipment will arrive on campus in January and thus allow us to carry out these experiments locally and with substantially less calibration overhead than our previous attempts.

Using a raster technique, we were able to graphically identify the vibrational modes encountered; this confirmed that our main measurements were of the fundamental (1,1) resonance mode. Furthermore, there exists another higher order resonance frequency (3+1) that cause what was believed to be an inconsistent and inexplicable set of measurements.

Design of Multiproduct Reactive Separation Plants

Students: Scott Turnberg (PhD, starting Jan 2005)

BACKGROUND:

Reactive distillation is a multifunctional process combining product conversion and separation inside a single piece of equipment. While the process has been demonstrated to significantly reduce both the capital and energy cost for highly non-ideal physiochemical systems, systematic design methods for generating and comparing design alternatives have been slow to evolve.

This projects seeks to combine recent analytical and algorithmic advances in the theory of reactive separation systems with the design of multiproduct plants for flexible production of acetate and oxygenate series. The main deliverables of the project will be:

(a) an algorithm capable of rigorously determining whether a particular set of reaction and separation tasks may feasibly take place in a single piece of equipment,

(b) a multi-objective optimization approach to assessing the economic trade-offs between the design alternatives generated,

(c) extensive case studies on current sequential and integrated processes to identify the first generation of pilot plant experiments for multiproduct equipment.

It is a goal to carry out the systematic search for solutions in part (c) using the agent system.

PROGRESS

Scott has spent most of the Fall semester analyzing pinch point bifurcation diagrams for the production of TAME; a four component systems with two independent chemical reactions. Using his own Matlab code -- and Aspen for verification -- he has compared a conventional reactor+column design with optimized alternatives for a fully reactive column as well as a non-reactive column with a sidedraw recycle to a pre-reactor. While clearly the most complex alternative, the side-draw solution appears to have advantages in terms of both capital and energy. Note that the amount as well as location of the column side draw -- and feed redistribution -- have to be carefully controlled. These answers are provided by the new method for analyzing feasibility in systems with disjoint feasible regions.

A visitor, Rui Filipe from Lisbon (Portugal), has also been using feasible region for optimal design of reactive distillation columns. Based on the concept of capacity variables -- developed by Megan Jobson at UMIST -- he has written an algorithm combining feasibility analysis in Matlab with NLP optimization in GAMS to identify the tradeoff surface between column size, reactive holdup and energy requirements for single-reaction systems with ideal VLE. Case studies are in progress and extensions to (simple) non-ideal systems are being planned.

On the implementation side, Scott has written a MEX interface to Auto2000 for bifurcation analysis and is working on the same for Multifario; a package for tracing out bifurcation hypersurfaces.

Erik Ydstie's Group

Modeling and Control of Particulate Processes

Student: Christy M. White (Ph.D.)

This research addresses modeling and control of yield and size distribution in particulate processes. We use a novel method for solar-grade silicon production, the thermal decomposition of silane gas in a fluidized bed reactor, as a benchmark. We have developed a model and control scheme for the behavior of particles in a fluidized bed reactor based on silicon production. The model simulates growth of silicon particles with ordinary differential and algebraic equations that track particle movement through discrete size intervals. The model solves quickly and is easily tuned to fit experimental data. The passivity-based inventory controller maintains a constant mass of a specified size of silicon particles. The results from this research will be published in Powder Technology.

This last year we have matched the model to pilot-scale process data obtained from Solar Grade Silicon LLC in Moses Lake, Washington. We developed an observer for on-line estimation of process states and parameters. The method allows for estimation of particle size distribution in real time. These results were presented at the AIChE meeting in Cincinnati. We have combined the observer based modeling scheme with inventory control for total mass and seed-mass control for on-line stabilization of the particle size distribution. Some results from this research will be presented at the Particle Technology Conference in Florida in May. The model and control scheme is being used for scale-up and control system design for production system under current development at SGS. It expected that that when the new process is in operation that it will provide several competitive advantages relative to the current Siemens process, including higher throughput per process unit, lower capital cost and significantly lower energy usage.

Modeling and Control of Distributed Process Networks

Student: Kendell Jillson (Ph.D.)

We have introduced a novel modeling framework for studying dynamics, distributed control, and optimization of complex chemical process networks. We are interested in developing distributed control systems that self-organize so that stability and optimality follows as a consequence of how the networks are put together and how they are connected with boundary conditions or other networks.

By considering only the topology of the system, basic conservation principles and the second law of thermodynamics we have developed a multi-component analog to Tellegen's Theorem of electrical circuit theory. This result has been combined with the passivity theory of nonlinear control. It is shown that under certain convexity conditions the network converges to a stationary solution. Under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized. Kendell presented this work in July at the 16th IFAC World Congress in Prague and at the AIChE meeting in Cincinnati.

We have also developed a theory for plant-wide control and stabilization of complex process systems. We have developed structural conditions for stability and simulated a recycle-flowsheet with a reactor and distillation column. The paper describing these results have been submitted for review in the Int, Journal if Process Control. We have used the network modeling theory to develop a networked model of the biological process of angiogenesis, the growth of new blood vessels. This is signaled by cancerous tumor cells as a way for tumors to increase their uptake of nutrients from the body as they grow. By modeling this problem with our network framework, we hope to gain insight into the system and eventually be able to suggest an optimal treatment strategy for dealing with tumor growth.

Real Time Optimization by Extremum Seeking Control

Eduardo J. Dozal-Mejorada (Ph.D.)

Wayo (Eduardo) has developed an online optimization technique for unconstrained optimization based on extremum seeking control. The optimization algorithm behaves as a stand-alone module using existing process models to gather information and adaptively drives the process to its extremum without altering the simulation code. The optimizer uses a second order approximation to a high order system and takes a set of modified equality constraints constructed so that they have the same geometric characteristics of the true steady-state behavior of the process. The module employs a dynamic model to obtain a steady-state model of the system. The steady-state model is then used to find the optimal input to the process. The optimum point obtained by the optimizer is tracked throughout process operation. The advantages of this adaptive algorithm over other traditional optimization approaches include: 1) it uses current process models, 2) it can handle multiple objective functions, 3) it only applies a subset of all process states, 4) it self-learning, and, 5) it is appropriate for steady-state or dynamic models. We have developed theoretical convergence and stability results for the exact-matching case and have started working on the robustness problem. Successful implementation has been applied to two case studies: 1) optimization of biomass production in a bioreactor, and, 2) optimization of silicon production in a reactor. These results were presented at the AIChE meeting in Cincinnati.

Wayo and Kendell have developed a method for optimization of complex supply chains using Kendell's network theory. They show that by focusing on value added and cost minimization in a distributed supply chain it is possible to achieve global optimality without a central coordinator if the activity rates are positive,

Passivity Based Control of Multi-Phase Reactor Systems

Student: Yuan Xu (Ph.D.)

The focus of this research is on passivity-based control of multiphase systems with reaction transport (diffusion and convection). To study this type of system, a metallurgic process has been chosen involving the carbothermic reduction of aluminum. This process takes carbon and aluminum oxide feed to produce aluminum. Work thus far has included developing a model using MATLAB to describe a variation of this process, as is being created by ALCOA, the world's largest aluminum producer. Proportional control is currently being used to explore the controllability, stability, and sensitivity of the system. Future work will be directed toward interfacing the FACT thermodynamics program with MATLAB via a MEX Interface. This will allow for the model to handle ranges of temperatures and compositions without extra work needed to determine equilibrium constants, activity coefficients, and extent of reactions. Another future improvement will be to incorporate computational blocks using the SIMULINK tools in MATLAB. Not only will this give the model a more "user-friendly" interface, but it will also allow for the exploration of modular simulation, where numerous monolithic simulation blocks can be combined and individually interchanged or altered without major recoding needed to modify the overall model.

Thermodynamics and Process Networks

Students: Luis Antelo (Ph.D. Univ of Vigo, Spain)

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.

Luis has continued Felipe's work on the flash systems stability and he is currently studying how he can extend these to distillation by combining his ideas on using the Gibbs-Duhem equation with the algebraic methods of Chad Farschman and the Lagrangian/Eulerian decomposition of Duncan Coffey. He has also developed a new theoretical framework for plantwide process control which we are currently testing in simulations. Luis went back to Spain in the beginning of December. He will come back to visit us for three months next fall.

Modeling the Vapor Recovery Reactor in Carbothermic Aluminum Production using Multi-Scale Modeling Methods

Student: Mohit Aggarwal (co-supervised with Prof Lee White) (Ph.D.)

Mohit just joined the group in November. He will start out his PhD by developing a model for the vapor recovery section of the carbothermic aluminum process under development by ALCOA. In this process aluminum is produced in a high temperature (2000C) two stage process. A significant amount of aluminum vaporizes from the aluminum reactor and this aluminum must be recovered in a vapor recovery column in order to maximize the production yield and save energy. We will model the primary reaction in the column, the gas flows as well as solid transport. The focus is to develop efficient methods to represent the thermodynamics and the multiphase behavior of the VRR. This work is a continuation of Vianey's modeling work (PhD/PostDoc 2004). Mohit will develop a three phase (liquid/solid/gas) multi-scale, simulation model which will be used for system design, scale-up, economic evaluation and control studies.

Adaptive Control using Selective Memory

Student: Priyesh Thakker (M.S.)

Priyesh joined the group in November. He will test a novel method for selective memory in adaptive control in simulation and pilot plant studies starting in January. He will focus attention on control of a steam water heat-exchanger in the unit operations lab at Carnegie Mellon. The method he investigates uses a newly developed technique to decide whether new data are informative or not by using a dual model adaptation concept which was subject to a patent application from CMU in May of 2005.

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