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GENERAL NEWS

Professor Il Moon from Yonsei University in Korea and Professor Maria Teresa Rodrigues from the University of Campinas in Brazil will be spending their 1999-2000 sabbatical leave in the Department of Chemical Engineering. Professor Moon, who is former student of Gary Powers, is active in the area of verification and discrete event simulation. Professor Rodrigues works in the area of scheduling. Iiro Hajuronski from Abo Akademi has joined Ignacio Grossmann's research group.

Dr. Juan Reyes, Assistant Professor from the University of Alicante in Spain, has joined the research group of Ignacio for a period of 6 months. Juan will be working in the superstructure optimization of extraction systems. Hector Yeomans successfully defended his Ph.D. thesis late in December. He has joined the office of McKinsey in Mexico City.

Arturo Cervantes, former student of Larry, completed his Ph.D. in February and has joined Mitsubishi Chemical Corporation. Kentaro Yasuda completed his MS degree and returned to Mitsubishi Chemicals in Japan. Dr. Dilek Alkaya has taken a position in the Chemical Engineering Department at the University of Alberta and Dr. Guillermo Sentoni has returned to Argentina as a research investigator at PLAPIQUI in Bahia Blanca, Argentina.

New Ph.D. students that have joined our research groups are as follows: Ling Jiang and Arvind Raghuanthan will be working with Larry Biegler, Christos Maravelias with Ignacio Grossmann, Warren Hofmaster, Gogi Singh and Vikas Verma with Steinar Hauan, and Dimitrios Gerogiorgis with Erik Ydstie

NEW MEMBERS

We would like to welcome Neste Oy as a new member of the CAPD consortium. The representative for Neste is Dr. Mauri Sourander. As with all of our members we look forward to rewarding research interactions with Neste.

IGNACIO GROSSMANN ELECTED TO NATIONAL ACADEMY OF ENGINEERING

It is a great pleasure to announce that Ignacio was elected to the National Academy of Engineering at their recent meeting. This is in recognition of Ignacio’s pioneering efforts in Mixed Integer Nonlinear Programming and its widespread applications in process synthesis, planning, scheduling and design and analysis under uncertainty. Ignacio joins Art Westerberg, Herb Toor and John Anderson as NAE members in the Chemical Engineering Department. Congratulations on this well deserved honor!

2000 ANNUAL REVIEW MEETING

Our Annual Review Meeting was held on March 27-28, 2000, and was attended by 35 participants from the member companies. The first day of the meeting consisted of overviews given by Art, Ignacio, Larry, and Erik, and was followed by a poster session by the students. On the second day the last year students gave presentations. This was followed by a discussion with industrial participants. The feedback we received was extremely positive. If you have any additional thoughts or suggestions, please let us know. Our next CAPD Annual Review Meeting will take place on March 26–27, 2001.

SUMMER SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* has taken place on June 22-28, 2000. There were 19 participants, with eight from CAPD consortium member companies and eight from outside the US (Mexico, Brazil, Portugal, Spain and Norway). We partitioned the six-day course into three modules:

a) Process Modeling and Synthesis - to be taught Thursday and Friday (June 22-23), focused on equation oriented systems, nonlinear programming and mixed- integer optimization.

b) Process Synthesis - to be taught on Saturday and Monday (June 24-26), will focus on conceptual insights and mathematical programming models for the synthesis of process flowsheets, with emphasis on reaction, separation and heat integration.

c) Process Operations. To be taught on Tuesday and Wednesday (June 27-28), will focus on differential/algebraic models for real time optimization and parameter estimation, and on mixed-integer programming models to process scheduling.

Each day included a workshop in which participants had hands-on experience with software and/or with solving relevant problems that emphasized the concepts we presented. Everyone reacted very positively to the obviously very busy schedule. Each participant left with much heavier baggage that included our extensive notes, the GAMS software, documentation and case studies, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in finding out more about the course, please contact Toni McIltrot at 412-268-3573, or e-mail: tm21@andrew.cmu.edu

WEBSITES/PROCESS SYSTEMS DIRECTORY

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

CAPD REPORT SERIES

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

EXECUTIVE SUMMARY

Highlights of **Larry Biegler's group** include further development of the reduced Hessian SQP (rSQP) strategy along several directions. The FORTRAN version of the rSQP strategy has been used for optimization of black box units including BVP solvers for dynamic systems and distillation columns. Problem classes that can be considered with this implementation will include data reconciliation, realtime optimization, and NLP sensitivity. Currently, **Andreas Waechter** is developing and refining barrier (interior point) NLP method based on many of these SQP concepts. This has been used to solve problems

with over 80,000 variables. In parallel to this effort, **Roscoe Bartlett** is developing a C++ environment for rSQP that incorporates a number of specialized decomposition strategies. Both are described below.

In addition, **Yi-dong Lang** has developed a user-friendly version of the dynamic optimization methods of **Arturo Cervantes**. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called DynoPC, runs under Windows with a GUI interface. It has been distributed to several CAPD members and can now be downloaded through an ftp server. Please contact lang+@andrew.cmu.edu or biegler@cmu.edu for more information. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package will be enhanced further by incorporating the ESO CAPE-OPEN modeling standards currently used in gProms.

In the area of reactor network synthesis, **Bill Rooney** has modified the flexibility approach of Grossmann and coworkers to deal with uncertainty associated with model parameters. This strategy incorporates nonlinear confidence regions into the uncertainty description in an efficient way and leads to a more realistic characterization of the impact of model uncertainty. Also, a novel way to generate bounds on these solutions has been developed using attainable region approaches. Finally, **Guillermo Sentoni** has demonstrated the use of efficiently derived neural network models for approximating the performance of optimal control problems. Along with our dynamic optimization strategies, this leads to a very fast implementation for nonlinear MPC and has been demonstrated on a number of real world problems.

The most relevant developments in the work of **Ignacio Grossmann's group** have been the following:

In the area of process synthesis **Jennifer Jackson** has extended disjunctive optimization models for distillation by Hector for the case of reactive distillation. Her models determine the number of stages, feed tray locations, and reactive trays. She has been testing her method in the production of ethylene glycol from ethylene oxide and water, and the metathesis of 2-pentene to form 2-butene and 3-hexene. **Juan Reyes**, a visitor from Spain, has initiated work in the area of superstructure optimization for liquid-liquid extraction.

In the area of optimization **Sangbum Lee,** has started to develop a branch and bound method for the global optimization of generalized disjunctive problems that involve nonconvex functions (bilinear, linear fractional and concave separable). He has applied this method to the global optimization for the synthesis of multiproduct batch plants in which a major decision is the assignment and integration of tasks to equipment. Sangbum has also completed the work for generating all the alternate solutions of an LP model using a recursive MILP formulation that was applied to the optimization of a metabolic network in collaboration with Professor Domach. **Aldo Vecchietti**, has been able to make further developments in the new version of LOGMIP for handling disjunctions through the use of IF ..THEN.. statements. .

In the area of planning and scheduling, **Iiro Harjunkoski** has developed an integration scheme for MILP and constrained logic programming (CLP) for the trim loss problem, which gives rise to an MINLP problem, achieving order of magnitude reductions in CPU time in the larger problems. Iiro has also developed in collaboration with Kvaerner a decomposition strategy for a large-scale scheduling model for steel manufacturing. The decomposition relies on grouping orders in smaller sets, which are first solved as a flowshop problem, and then joined through a jobshop MILP formulation. This has allowed Iiro to solve problems with more than 100 orders. **Jayanth Balasubramanian,** has been developing a rigorous solution method for minimizing the expected completion time in flowshop plants with uncertain processing times. Since the method described in the previous newsletter applies only for plants with two stages, Jaynah has developed a branch and bound method that makes use of partial schedules that involve average processing times for unassigned jobs, which provides a rigorous lower bound. **Sarette Van Den Heever**, who has been working in the planning and design of offshore oil field facilities, has developed a novel Lagrangian decomposition method for incorporating royalties in the optimization of these systems, an objective function which greatly increases computation time. She has been able to solve a problem with 16 well platforms and 23 pipe interconnections over 15 time periods, which previously could not be solved after 5 days of CPU time. **Christos Maravelias** has initiated his research in the area of simultaneous product

testing and design and planning of batch manufacturing facilities, a problem that arises in pharmaceuticals and agricultural chemicals. In the area of supply chain optimization, where Ignacio has collaboration with Erik Ydstie, **Edgar Perea** has developed a dynamic model for a manufacturing-distribution-retail system, and implemented it in MATLAB. Different control policies for inventories and order placements can be readily studied with this system. Finally, **Fabian Valli** has ported most of the MILP/MINLP interfaces to the PC.

Steinar Hauan's group started up in January of 2000 with 3 Ph.D. students and 1 MSc student. The research aims at expanding the scientific basis for design and operation of complex chemical processes through mathematical analysis, geometric visualization and verification by numerical simulations. Special focus is directed towards development of engineering insights in order to produce solutions that are well understood.

A main research branch involves hybrid or multifunctional units with emphasis on expanding the ideas around our recent publications on generalized difference points. **Warren Hoffmaster** will focus on the feasibility of reactive separation processes, i.e. attempt to identify the proper limiting conditions in processes where reaction and separation takes place inside the same piece of physical equipment. **Vikas Verma** will adopt a different view and work on conceptual and economic analysis of flowsheets with the goal of comparing simultaneous and sequential reaction and separation. Work has been started on implementation of bifurcation, thermodynamics and collocation methods.

Gogi Singh will look into the area of miniature process devices with special emphasis on architectures for biological sensor and high-throughput screening systems. The main idea is to analyze how the effect of special scaling and control issues affect traditional synthesis algorithms. Work on numerical simulation of microscale fluid flow and mixing has been initiated. The last addition to the group is **Murni Ahmad** who will be working in collaboration with Todd Przybycien's group on the design of biochemical and pharmaceutical processes with multiple time horizons. The initial focus on operation of condensation reactions and protein separation.

Two of **Art Westerberg's** students completed their Ph.D. projects this last May: **Jae Woo Lee** and **Russ Milliken**. Jae prepared one new paper, which analyzes the MTBE and ethyl acetate reactive distillation processes graphically. He shows that one can quantitatively predict an optimum reflux ratio to use in the latter process using a graphical projection method. Russ completed his work on the notification server AWARE. He attached it to the LIRE' document management system and tested its use in two general engineering design courses. This system can easily expand to handle an increased number of events and uses itself to make the system reliable.

Lifei Cheng continues his work on the creation of a simulation capability for to handle stochastic models. He is looking at how to assess the vulnerability of a process to future technological breakthroughs. His latest work is to study recursive model formulations for such problems.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

Large Scale Optimization Strategies

Students: **Roscoe Bartlett (Ph.D. student started Fall, 1996)**
Gregory Itle (Ph.D. student started Fall, 1998)

Roscoe Bartlett is developing and testing an object oriented version of rSQP written in C++. This version allows the easy incorporation of options, Hessian classes, different linear algebra and QP solvers, as well as dynamic memory allocation and management. This approach makes extensive use of mixed language

programming so that the 'number crunching' parts are handled by FORTRAN (and mostly BLAS) routines while the higher level code is in C++. To do this work, Roscoe has developed a comprehensive structure for linear algebra.

In addition, Roscoe has developed rSQP methods based on the application of Schur complements for the active set strategy in the QP. This approach has been very successful for the SOCS code at Boeing. Unlike the QPKWIK algorithm, the application of Schur complements allows us to directly exploit the structure of the entire KKT matrix at the linear algebra level. As a result, a general active set strategy can be developed for very efficient NLP algorithms for rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization.

When applied to standard NLP test problems, this new QP approach is about three times faster than QPKWIK. Moreover, it allows us to develop more flexible NLP strategies that deal with smaller reduced Hessians, better exploitation of sparsity and changing active sets. These features are similar to those in CONOPT but here we apply them in an infeasible path mode. Finally, the resulting strategy fits well with the object oriented construction of the program and also serves as a nice complement to the barrier strategies discussed below. In fact, our goal is to identify problems where different problem classes can exploit various SQP options. For this purpose, we have considered large dynamic optimization problems for NMPC and would like to know when barrier approaches are favored over active set strategies. We have applied both approaches for the full-scale Tennessee Eastman problem and noted the following features:

- for problems with many states and few controls, a reduced space approach has significant advantages over NLP methods with full space decomposition. This is often due to limitations of current sparse linear solvers

- for problems with few active constraints a well implemented active set strategy still has advantages over barrier methods. These advantages disappear as the number of active constraints increases.

Preliminary results of this comparison are described in an ACC paper listed below. More extensive results of this comparison will be presented at the ACC meeting at the end of this month.

Gregory Itle is extending these rSQP ideas into the area of optimization of systems described by partial differential equations. Working with researchers at Sandia National Lab and with Prof. Omar Ghattas and his group, he is applying NLP strategies to finite element models for fluid flow and elasticity. He has developed a prototype interface of rSQP code with MP SALSA, a large-scale partial differential equation solver. This was demonstrated on the optimization of a natural convection system. Currently, he is streamlining the rSQP FORTRAN code to adapt it to larger NLP problems. For this topic Greg is also looking at constraint aggregation strategies that allow much less overhead to constraint activity and also allow conventional QP solvers to be used even if there are millions of bound constraints. Greg is spending the summer at Sandia to implement and test these ideas. He will be joined by Roscoe and Larry in August for the last two weeks of his stay.

Barrier (Interior Point) Methods for Nonlinear Programming

Students: **Andreas Waechter (Ph.D. student started Fall, 1997)**
Faculty: **Prof. Reha Tutuncu, Department of Mathematics**

This project extends the previous project by developing an efficient strategy for solving nonlinear programs, generated by rSQP, with interior point (IP) methods. This approach works either in the full space or can take advantage of the particular rSQP decomposition (choices of Z and Y). However, it solves the nonlinear problem directly without first exploring the solution of the QP subproblem. In this way we avoid the overhead in solving highly constrained QPs, as these have the same level of combinatorial complexity as the original NLP problem. A paper that describes our earlier work in this area (by Ternet) is listed below.

Working with Prof. Tutuncu in the Math Department and with Prof. J. Nocedal at Northwestern, we are considering the direct solution of the NLP with barrier methods. This approach will first be applied to problems that allow positive definite reduced Hessian approximations. This eliminates the need for calculating second derivatives of the objective function or from the model equations. Here we are adapting the algorithms of Byrd and Nocedal to specialized characteristics encountered in process engineering optimization problems. A number of variations to this approach have been developed and tested that include the use of trust region and line search approaches, decoupling the barrier terms from the reduced Hessian approximation and options for both primal and primal-dual barrier terms. Here a FORTRAN code has been implemented for the solution of dynamic optimization problems; problems with over 55,000 variable problems were solved in under 11 CPU minutes on a 400 MHz computer. A paper that describes this approach in detail along with results on these dynamic optimization problems is listed below.

More recently, Andreas has discovered that Newton-based IP methods that are applied directly to NLPs can experience convergence failures. These failures are analogous to infeasible QPs that can be encountered in SQP but are much more subtle because the cause cannot be detected easily. In particular, Andreas has developed a counter-example that illustrates this problem, and has also developed a through analysis of this difficulty. He has also shown that trust region approaches, as developed by Byrd, Nocedal and coworkers, do not suffer from this difficulty. Because barrier methods have seen considerable activity in the optimization community, this example has attracted a lot of attention in the Math Programming community. Andreas has also developed an improved line search algorithm that overcomes this convergence difficulty and has completed a rigorous global convergence proof for his approach. Numerical testing has also shown some significant performance improvements over other barrier algorithms. Andreas is spending the summer at Northwestern University to work with Prof. Nocedal on further extensions of this approach.

Optimization of Differential-Algebraic (DAE) Systems

Students: **Arturo Cervantes (Ph.D. started Fall, 1995)**
Arvind Raghunathan (Ph.D. started Fall, 1999)
Researcher: **Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**

This project deals with simultaneous solution and optimization strategies for large-scale, dynamic optimization problems. We have applied this approach to optimization problems for batch reactors, process dynamics and tray-by-tray batch distillation and large-scale dynamic flowsheeting models. Moreover, we have tackled dynamic examples successfully with this approach that cause any sequential dynamic optimization method to fail. This is due to the possible presence of unstable modes in the forward direction. It can occur in open-loop unstable systems that arise in optimal control and nonlinear MPC, dynamic parameter estimation and the optimization of runaway reactors. This approach can also be integrated into a two level optimization strategy that alternately solves the dynamic optimization problem for a fixed mesh, and then optimizes the mesh in an outer level. This approach easily allows for the addition of finite elements as well.

Arturo Cervantes completed his Ph.D. last February. In his thesis, he developed and expanded the simultaneous approach to solve moderately large dynamic optimization problems. This is being accomplished through the incorporation of more efficient matrix decomposition strategies, with COLDAE routines to set up the collocation equations. Arturo has developed and demonstrated the efficient solution and optimization of these systems with MA28 and MA48. In addition, Arturo has solved a number of process optimization problems including the dynamic optimization of reactive distillation columns, polymerization reactors and crystallization units. Recently, Arturo has been involved in two areas. First, he is working with Dr. J. A. Bandoni and his colleagues at PLAPIQUI in Bahia Blanca, Argentina to refine an optimization model for a LDPE reactor. The dynamic optimization problem deals with shortening the grade transition time from one set of operations to another. Application of the above strategy led to an optimization of a DAE model with over 200 DAEs in less than 10 CPU minutes. As a result, the transition time for this reactor was shortened from five to two hours. This model has also been extended to incorporate reactor kinetics and consists of over 530 DAEs. Arturo has also developed an element-by-element decomposition of these collocation equations, using stable pivoting strategies. With this approach,

he has considered difficult dynamic optimization problems for very large process models, that would otherwise exhaust the storage requirements of our computers. As part of this work, he is working with Andreas Waechter and has implemented the interior point methods of Byrd and Nocedal to expedite the handling of inequality constraints. As described in above, these have led to very efficient optimization strategies and have led to another doubling of performance over the best rSQP strategies. The results of this approach are described in the paper listed below. The results of the LDPE dynamic optimization will be presented at the PSE 2000 meeting this summer and will be listed in the next newsletter.

Moreover, Arturo has extended this interior point approach to include the placement of finite elements during the convergence of the optimization strategy. The nested approach of the interior point strategy allows the addition of moving finite elements at various levels. Thus, we can converge the overall dynamic optimization problem with moving finite elements in an efficient and robust way. Here the key idea is that barrier problems are solved to increasingly tighter tolerances, at which an increasing number of finite elements can be relaxed. Moreover, within the barrier problem, the influence of the element is differentiable - this avoids the problems associated with earlier algorithms. To illustrate this aprpoach, Arturo has solved several large-scale examples in his thesis, including the LDPE problem described above.

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

Finally, Arvind Raghunathan has begun to work on dynamic optimization and the use of complementarity constraints in optimization problems. This allows us to build on the efforts of Arturo and Andreas, both in barrier methods and dynamic optimization. A key advantage is that complementarity constraints can be handled directly and simultaneously with interior point methods. This allows us to deal with problems that require conditional relations including phase equilibrium and disappearing units.

Dynamic Optimization Strategies using DAE Solvers

Students: **Karl Bloss (Ph.D. student at Lehigh University)**
Ling Jiang (Ph.D. started Fall, 1999)

In tandem with the above project, we are also developing more direct sequential strategies for the solution of dynamic optimization problems. These approaches are better known and have seen a lot of previous development. They have disadvantages for unstable systems encountered in reactive and control systems but incorporate very efficient DAE integrators that are well-suited and well-tested for dynamic simulation. An additional bottleneck is obtaining sensitivities from the dynamic model efficiently. Fortunately, recent projects by Barton at MIT, Petzold at UC-Santa Barbara, and researchers at the Max Planck Institute have led to excellent software implementations that calculate sensitivities efficiently from large DAE process models. As a result, we are embarking on large-scale dynamic optimization projects that combine our large-scale rSQP tools with efficient DAE solvers and sensitivity codes.

In a joint project with Prof. Schiesser at Lehigh University, Karl Bloss is developing dynamic optimization strategies for the startup and dynamic analysis for air separation units. These systems are tightly coupled and need to adapt to many changes in operation cycles. As a result, off-spec product and transition times need to be minimized efficiently. For this project we are developing and reformulating large-scale, high index models and adapting our optimization strategies to deal with them. One interesting approach has been the use of adjoint strategies for the calculation of sensitivity information. This approach is well suited to

problems that have many degrees of freedom and few constraints. To exploit this feature we have applied several constraint aggregation techniques and incorporated these into the dynamic optimization problem. As a result, the adjoint technique can now be applied with significant savings over direct sensitivity approaches. Karl has demonstrated this approach on a number of dynamic optimization examples.

Related to this project, is a new GOALI initiative with Air Products for the optimization of Pressure Swing Adsorption (PSA) systems. For this approach we intend to exploit existing models and implementations for the optimization of comprehensive, detailed PSA systems. Ling Jiang has begun to work on this project. She is spending the summer at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, to adsorption bed models created from the method of lines. Using this approach, new algorithms will be developed for cyclic steady states and optimization of design parameters for PSA systems.

Synthesis of Reactor Networks for Waste Minimization

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

Synthesis of optimal reactor networks directly affects all downstream activities and has important implications on separation sequences, energy management and integration and waste minimization. Our previous work dealt with application of geometric principles for defining an attainable region for the reacting system. Here, many literature examples were solved in a simple manner with much better solutions than reported previously. This approach readily deals with arbitrary kinetics and extends naturally to general nonisothermal systems. In general, our approach requires the optimization of Differential-Algebraic systems, but these are not particularly difficult because of our collocation based formulations. An additional advantage to this approach is that it has been integrated within a process flowsheet model so that targeting can be performed for the reactor, with consideration of other aspects of the process, such as heat integration and separation systems.

In particular, our research extended attainable region concepts to more complete MINLP formulations that overcome some of the deficiencies in previous optimization formulations. This has led to a simple superstructure that also incorporates the properties of differential sidestream reactors (DSRs) with optimized sidestreams, which can become important for higher dimensional representations. This approach achieves results that are as good or better than previous studies and overcomes many of the obstacles observed with these studies. To continue this work, we have interacted heavily with Prof. Glasser’s group at the University of Witwatersrand. In particular, Brendon Hausberger visited with us last fall to continue this interaction. The results of his visit led to a close synthesis of optimization and geometric methods for targeting attainable regions for reactor networks and an algorithmic approach for the construction of attainable regions for reactor networks. This approach is optimization based and deals with the development of lower dimensional projections that can be combined to obtain the full dimensional region. A paper that describes this approach will be presented at PSE 2000 and will be listed in the next newsletter.

Since then, Larry has also visited Prof. Glasser's group in South Africa. This visit led to prototype concepts for algorithmic generation of attainable regions. Shehzaad Kauchali will be joining us this summer to continue this work. We intend to apply large-scale optimization to convex problems to generate these regions. Preliminary results show that this approach is quite encouraging - and can be generalized to a number of multi-dimensional problems.

Moreover, Bill has developed a framework to assess the design or reactor networks with uncertain kinetic and process parameters. A paper that describes this approach is listed below. This approach incorporates joint confidence regions obtained from experimental data within the reactor design problem as well as other process problems. Use of these regions leads to an approach related to flexibility analysis with some additional structure that can be exploited for efficiency. This approach leads to a multiperiod formulation with additional feasibility tests.

This approach has also been extended to uncertainty associated with reactor networks. Here the multiperiod approach employs both AR concepts to generate bounds as well as solution of the MINLP superstructures to develop excellent candidate solutions. The approach has been applied to a variety of process problems and will be listed in the next newsletter. Bill is currently refining this approach to deal with nonlinear confidence regions. While these are more difficult to generate, especially for larger problems, the confidence regions can be significantly different than for linear models and their impact of robust designs can also be quite different. Bill has developed a number of examples that illustrate this difference. Results of this approach will be described in the next newsletter.

Data Reconciliation for Steady State and Dynamic Processes

Students: **Nikhil Arora (Ph.D. started January, 1999)**

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

Following up on the work of Dr. Joao Albuquerque, Nikhil is investigating the Fair function along with a number of redescending functions by Hampl and others. These approaches have the advantage of providing simultaneous outlier detection while at the same time yielding less biased estimates of the reconciled data. Nikhil has benchmarked a number of M-estimators on several literature examples. Preliminary results show that the power (recognition of outliers) is as good or better than with more expensive approaches and that the detection of false positives is also largely avoided. Nikhil is currently refining this approach and compiling these results in a paper that will be presented at the next AIChE meeting.

<u>Ignacio Grossmann's Group</u>

Systematic Framework for the Representation and Modeling of Separation Synthesis

Students: **Hector Yeomans [Ph.D., Jan 96-Dec 99]**
Jennifer Jackson [Ph.D. , started Jan 99]
Visitor: **Juan Reyes [postdoc, started June 00]**

New development: *Tray-by-tray model for reactive distillation by Jennifer Jackson*

Summary Hector's Ph.D. work.
This project was part of the GOALI project with Jeff Siirola and Art Westerberg, and has as an objective to provide a fundamental framework for the synthesis of process flowsheets through the mathematical programming approach. The first focus was on representing superstructures, and developing optimization models using disjunctive programming as the underlying framework. The overall modeling framework consists of the following steps:

1. Develop a superstructure for either of the two representations:
a) State-Task Network (STN) that consists of two types of nodes: states and tasks. The assignment of equipment is dealt implicitly through the model.
b) State Equipment Network (SEN) that consists of two types of nodes: states and equipment. The tasks in this case are treated implicitly through the model.

2. Develop a generalized disjunctive programming (GDP) model. The model for the STN involves multiple terms defined over the equipment. In contrast the GDP model for the SEN representation involves for each task, disjunctions with multiple terms defined over the tasks.

3. a) For the linear case, reduce the model of step 2 into an MILP.
   b) For the nonlinear case the problem is tackled directly with generalized disjunctive programming algorithms.

For the case of linear distillation models, Hector developed GDP models, and was able to systematically derive the MILP proposed by Andrecovich and Westerberg model.

In order to handle heat integration in distillation problems, we collaborated with Zdravko Kravanja to develop a disjunctive programming model for simultaneous optimization and heat integration. The model also relies on the idea of pinch location as in Duran's model, but makes an explicit distinction between isothermal and nonisothermal streams, and produces rigorous results, whereas Duran's model fails for isothermal streams. . Hector used these models and tested them on several problems, finding that the major benefit was *greater robustness* in the optimization compared to traditional MINLP models. The proposed approach was also applied to a tert-Butyl Methacrylate flowsheet that has a distillation subproblem with 4 components. The simultaneous approach led to very significant savings compared to the flowsheet reported in the literature.

Hector also developed synthesis models based on tray by tray models. The feed, condenser and reboiler trays were treated as permanent rays, while the trays between the feed and the condenser and between the feed and reboiler were treated as potential trays, whose existence was modeled through disjunctions. Using GDP the NLP subproblem only deals with existing trays avoiding singularities. As for the superstructure of columns we rely on the SEN representation, which is in turn modeled as a GDP problem. Hector has shown that the initialization for any sequence requires only the solution of two NLP subproblems (upper and lower part of each column). He applied the tray-by-tray model to both individual column designs, and to the separation of an ideal ternary mixture. This work is reported in the reprint of the I&EC reprint that we enclose.

In the last part of his thesis Hector has addressed the synthesis of complex columns. The approach he took taken for developing the superstructures, which is non-trivial for these problems, is to use as a basis the recent STN representation by Sargent which can also be used for azeotropic separations. For the ideal case this superstructure reduces to the well-known Sargent and Gaminibandara superstructure. The basic idea is to map each of the tasks in the STN representation of Sargent as a column section. The interconnection of column sections is performed with permanent trays, which are generalized to perform different tasks (condenser, reboiler, feed) that are not specified a priori. The synthesis problem is formulated as a GDP model and solved with the modified logic-based outer-approximation method. This method was applied to a mixture of light hydrocarbons, to the separation of ethanol and water using methanol as an entrainer, and an industrial problem where several intermediate components are present in low concentrations. All these problems were successfully solved. The first led to a Petlyuk column design, the second to a column with a side rectifier, and the last to a single feed column. Since these problems involved several thousand variables computing times ranged from 1 to 3 hours. We enclose the paper that was a result of this work, and which we submitted for publication.

Jennifer Jackson-Reactive Distillation

Over the last few months Jennifer has been diverted from her retrofit project (see below), and has been addressing the optimal design of reactive distillation columns. Her work has used as a starting basis the disjunctive programming model developed by Hector. Jennifer has started with the optimal design of a column where the major decision involved are selecting number of trays, the trays where reaction takes place, and the number and location of feed trays. The basic idea in Jennifer's model is to consider all trays as being conditional. She also assumes reactions in the liquid phase to be described by kinetics. Currently Jennifer considers in the conditional trays that both reaction and phase equilibrium make take place, or else whether there is no mass exchange. At a future stage she will also explore three cases: no mass exchange, only phase equilibrium, both phase equilibrium and reaction. Her preliminary results include production of

ethylene glycol from ethylene oxide and water, with side reaction of ethylene oxide and ethylene glycol to form diethylene glycol. This problem has been reported before by Amy Ciric. The other problem Jennifer is working on is the metathesis of 2-pentene to form 2-butene and 3-hexene (specifically 2-cis-pentene, 2-cis-butene, and 3-cis-hexene). The major outcome so far has been the development of a fairly robust model and good initialization scheme, since the NLP subproblems in these problems are difficult to solve.

Juan Reyes: Liquid-Liquid extraction
Juan Reyes has only recently arrived and is in the process of developing superstructures for liquid-liquid extraction systems in which many interesting alternatives will be considered. For instance, number of stages, location of intermediate feeds and extractions, splits and selection of solvents.

Planning for Retrofit Design in Process Networks

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

Jennifer has left this project on hold due to her involvement in the reactive distillation project. This project is concerned with developing both high level as well as detailed optimization models for process modifications. At the high level Jennifer's problem can be stated as follows. Given is an existing network of processes for which process modifications such as improvement of yield, increase of capacity, or reduction of energy consumption and/or waste generation are considered over a period of several years. In each year there is a limit of capital investment for retrofit projects. The problem consists in identifying retrofit projects for those processes that will yield a maximum improvement in the Net Present Value. One of the challenges in this problem is how to estimate the effect of the various types of process modifications, without having to carry out a very detailed study in each plant.

Jennifer has developed a generic linear model for processes in which the various types of modifications can be incorporated. Tools such as attainable regions and pinch analysis are being explored to help estimate the benefits and limits of improvements. The problem is modeled as a multiperiod disjunctive programming problem that can be reformulated as an MILP. Disjunctions are used to select from among the several alternatives for process modifications. Jennifer has tested these ideas on a network with 5 processes that include processes for producing acetaldehyde, acrylonitrile, acetone, phenol and cumene. Jennifer considered a time horizon of three years, and possible modifications for improving the yield, increasing the capacity and increasing the energy recovery in each process. She formulated the problem as a multiperiod disjunctive optimization problem and reformulated it as an MILP problem. The solution predicted one modification for four out of the processes in the three time periods. It is interesting to note that when the problem was solved as a conventional MILP problem, it took 2300 secs versus the 18 secs of the GDP formulation.

Algorithms for Nonlinear Disjunctive Programming

Students: **Sangbum Lee [Ph.D., started Jan 98]**
Research fellow: **Aldo Vecchietti (Ph.D., started Jan 98)**

New development: *Global optimization algorithm for nonconvex disjunctive problems*

Sangbum Lee: Nonlinear GDP
The objective of Sangbum's project is to develop solution methods for generalized disjunctive programs involving multiple terms in the disjunctions, which are given in the form:

$$\text{Min} \quad Z = \sum_i \sum_k c_{ik} + f(x)$$

$$\text{st} \quad g(x) \quad 0 \qquad \text{(GDP)}$$

$$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(x) \leq 0 \\ c_{ik} = \gamma_{ik} \end{bmatrix} \qquad k \in SD$$

$$W(Y) = True$$
$$x \in R^n,\ c \in R^m,\ Y \in \{true, false\}^m$$

We have shown previously that a convex NLP relaxation model can be derived that is based on considering the convex hull for nonlinear convex inequalities. This NLP has the property that it gives tighter lower bounds than the ones that are obtained when the above GDP is converted into an MINLP with "big-M" constraints. This NLP relaxation can be used in three different ways:
I) To reformulate the above GDP as an MINLP, which can then be solved with methods such as outer-approximation, generalized Benders and extended cutting plane.
II) To develop a logic based outer-approximation algorithm in which the NLP subproblems only involve the active terms of the disjunctions, and where the MILP master problem is constructed by linearizing the NLP relaxation, as opposed to linearizing the functions themselves and then apply the convex hull.
III) To develop a specialized branch and bound method that makes use of the new NLP relaxation by branching on the terms of the disjunctions rather than on the 0-1 variables.

The reformulation and the branch and bound algorithm have been applied to various GDP problems, including problems related to process networks, optimal positioning of new products, and batch design. The main conclusion in all these applications is that significantly improved lower bounds were obtained in most problems compared to the traditional MINLP models, which often translated in more efficient solutions.

As described in the last newsletter, Sangbum has had a small but interesting diversion in his research. In collaboration with Michael Domach, a faculty from Chemical Engineering in the bioengineering area, he has been involved in the problem of finding all the alternate solutions of an LP related to a metabolic network. While there are a several special purpose methods reported in the literature for finding all alternate optima in an LP, there are no codes that are readily available for this problem. This motivated the development of an MILP formulation that can be applied to LPs with variables that are unrestricted in sign, and that may exhibit degenerate solutions. The proposed method has been applied to the LP of a metabolic network involving about 50 variables and constraints. Typically these problems involve between 10 and 30 alternate optima that our proposed method can rigorously find. We enclose a manuscript on this work.

Over the klast few months Sangbum has been developing a global optimization algorithm for solving Generalizd Disjunctive Programming problems involving nonconvexities in the form of bilinear, linear fractional terms and separable concave functions. Main idea behind the proposed method is to perform a branch and bound search with the convex NLP relaxation that results from replacing the nonconvex terms with convex envelopes, and applying the convex hull over the disjunctions that have not been selected. When feasible discrete solutions are found in the tree, the resulting reduced NLP subproblem is solved with a global optimization. In our case we have used a variation of Juan Zamora's and Ignacio Quesada's algorithms. Sangbum has applied this algorithm to several problems. The largest is related to the synthesis of batch processes in which the major problem consists in deciding what tasks are assigned to which equipment, with the possibility of merging tasks to reduce the number of equipment. Assuming zero-wait policy and single-product campaigns For a problem involving 6 tasks, 7 equipment and 6 products gives rise to a GDP with 53 boolean variables, 105 continuous variables and 13 disjunctions. The algorithm found the rigorous global optimum ($726,205) in about 2 minutes. In contrast, applying DICOPT to the MINLP formulation to that problem yields a suboptimal solution of $787,983. Sangbum is currently applying this algorithm to pooling and blending problems with fixed charges and semi-continuous flows.

Aldo Vecchietti: LOGMIP and modeling issues

The project by Sangbum is being complemented by Aldo Vecchietti in Argentina who will be submitting next month a Ph.D. thesis in Santa Fe, Argentina, based on this work having both Ignacio and Jaime Cerda as co-advisors. The man thrust of the work by Aldo has been the developments of LOGMIP, as well as the analysis of alternative models for disjunctive programming. Aldo has produced a PC version of a new version of the LOGMIP code, which is as an extension of the GAMS modeling language for posing logic/disjunctive problems. The main feature of the new version of LOGMIP are several language constructs in order to concisely formulate GDP problems. The syntax that he developed involves the use of IF THEN ELSE statements to represent the disjunctions. In each of these blocks of constraints can be specified. Aldo has recently show that the IF THEN ELSE construct can be applied to embedded disjunctions. An interesting development has also been to show that logic constructs that are commonly used in Constrained Logic Programming (CLP), such as implications for constraints (eg g(x) 0 => f(x) 0) can be systematically converted in the form of disjunctions. Therefore LOGMIP is able to handle implications by simply converting them internally into disjunctions. In fact one example from ILOG was totally transformed into a GDP and successfully solved with LOGMIP in one single iteration.

The logic can also be expressed in symbolic form, and a previous PROLOG program developed by Michelle Tourn is being used as a basis. The intent is also to be able to accommodate MINLP models in algebraic form, as well as hybrid models that are partly expressed as disjunctions and partly as equations.

The other important development in Aldo's current work is the implementation of the convex hull relaxation that has been studied by Sangbum, and that is used to reformulate GDP problems into MINLP problems. The major advantage of this approach is that it s quite general as it can be applied to general mathematical GDP formulations. Work is currently under way to allow in LOGMIP the choice of MINLP reformulation based on the convex hull, and the solution of the logic based OA algorithm by Metin Turkay. Finally, Aldo has also developed some interesting insights into the question as to when it pays or not to reformulate disjunctions as big-M constraints or as mixed-integer constraints based on the convex hull.

Scheduling of Batch and Continuous Multiproduct Plants

Student: **Vipul Jain [Ph.D. started Jan 1996]**
Postdoctoral fellow: **Iiro Harjunkoski (started September 1999]**

New Development *Novel scheduling strategy for steel manufacturing*

Vipul Jain: Integration MILP/CLP
Vipul's project dealt with a variety of issues related to scheduling. He first considered cyclic scheduling and maintenance of parallel units with decaying performance, and then short term scheduling of two-stage processes with intermediate storage. He also has addressed the resource constrained problem for new product development. Since all of these problems involved MILP models, Vipul also explored the use of constrained logic programming (CLP), which has been extensively commercialized by ILOG, the French company that recently purchased CPLEX.

The last part of Vipul's work dealt with the integration of constrained logic programming (CLP) and MILP optimization. CLP is essentially like Generalized Disjunctive Programming in that it uses disjunctions and logic constructs. The major difference is that the solution method relies on implicit tree search enumeration, combined with domain reduction and constraint propagation. Using ILOG in some problems (mostly discrete in nature), Vipul found that this code tended to outperform MILP models solved with CPLEX. However, in some problems ILOG was unable to solve problems in reasonable time.

Vipul developed an approach for the class of scheduling problems that can be characterized in terms of assignment and sequencing decisions, and in which the sequencing variables do not appear in the objective function. The point here is that when the assignments are fixed (e.g. each job assigned to given machine), then the remaining problem reduces to a feasibility problem, which traditionally is hard to solve with

MILP. So the idea is to solve the problem at two levels: (1) assignment level with MILP, (2)-sequencing level with CLP. The first level acts as a master problem and is updated with cuts derived from the sequencing subproblems. Vipul has applied this approach to a single stage/parallel lines problem, and in which jobs are specified with release and due dates. The objective is to minimize the assignment cost. Vipul solved "easy" and "difficult" versions for problems with different number of orders and parallel units. Both the MILP and CLP methods exhibited exponential behavior in that the largest problem (20 orders, 5 parallel machines) could not be solved to optimality after several hours. The integrated scheme in contrast required less than one minute to find the optimal schedule!

Iiro Harjunkoski: CLP/MILP for trim loss problem and novel strategy for steel manufacturing
Iiro has undertaken two projects. The first has been to continue te work initiated by Vipul Jain for integrating CLP and MILP. Initially, Iiro applied the idea to the trim loss problem, which is a MINLP problem where wide raw paper reels are to be cut into narrower product reels by minimizing the waste, as well as, some other production parameters such as the number of different patterns needed. The approach that Iiro developed was to linearize the MINLP by introducing new variables that correspond to products of discrete and continuous variables. This MILP corresponds to a relaxation that yields a lower bound, and often yields very good approximations of the original problem. At that stage the problem of finding a feasible solution with the original nonlinear integer constraints is reformulated as a CLP problem with a fixed value of the objective. If no feasible solution is found, the value of the objective is increased and the CLP is resolved until a feasible solution is found. The results of two examples (first one has 5 different product widths, in total 118 reels and the second one has 7 product widths and a total of 189 reels) are as follows:

Example	Binaries (SOS)	No. patterns (total/types)	CPU-seconds MILP	CLP	Hybrid
1	154	24/5	10843	8509	65
2	316	38/4	9884	>50000	52

Iiro has also been working on a scheduling problem for steel manufacturing in collaboration with Kvaerner. This problem contains a large number of chemistry-, geometrical- and scheduling rules which makes already a problem containing 10 heats practically impossible to solve by MILP. The production is therefore highly sequence dependent. Certain properties of the problem, e.g. the fact that the products need to be grouped for the last operation motivate a decomposition of the problem. The chosen approach will divide all orders into groups of 1 to 8 heats, then solve each group as a flowshop scheduling problem. This solution is then integrated into one production line by deciding the optimal sequence of the groups, which is equivalent to a jobshop scheduling problem. The final solution step, in which the heats are again handled individually, consists of an MILP including some equipment decisions and the final schedule is made more compact.

The resulting approach can schedule a one-week production (80-100 heats) within a few thousand CPU-seconds and the flexible structure of the strategy also allows rescheduling by solving only parts of the main problem. It should be noted that this corresponds to 6400-10000 binary variables in a basic job-shop scheduling approach. Furthermore, issues such as maintenance can be included in a natural way.

Uncertainty in the Scheduling of Batch Processes

New student: Jayanth Balasubramanian [Ph.D. started November 1998]

Status: New MILP for Flowshop Scheduling based on Semi-analytical Graph-Based Model

Jayanth's project deals with batch scheduling problems in which the initial uncertainties considered are processing times. The conceptual problem is to find a schedule that minimizes the expected completion time. As an initial step Jayanth has restricted himself to flowshop scheduling problems consisting of two stages and with no changeover times. Also, he has initially assumed discrete probability functions for the processing times.

The basic idea in Jayanths's approach for two-stage flowshop problems is to represent a fixed schedule as a directed graph. The expected completion time can then be computed by integrating over all possible paths the expected completion times. For the case of flowshop plants this integration can be simplified by decomposing the corresponding graph into series-parallel structures that lead to two node subproblems. The key extension of Jayanth's work has been to discover that these integrals can be written as a function of the assignment of jobs to the nodes with the use of 0-1 variables. In that way the problem of selecting the schedule with minimum completion time can be formulated as a nonlinear integer program that involves bilinear, trilinear and multilinear terms of the 0-1 variables. By performing exact linearizations of these terms, the problem can be reformulated as an MILP, which in general is of much smaller dimensionality than a multiperiod version of a deterministic scheduling MILP model. Jayanth has applied this method first to a batch plant with 4 products, 2 stages, in which there are 3 discrete probabilities for each processing time. If one were to use a multiperiod MILP approach the problem involves 6561 scenarios, and is modeled with 104,993 variables and 118,107 equations. Using CPLEX 6.5 this problem was solved in 2.8 hours. With Jayanth's approach the MILP only involved 436 variables and 1202 equations, and was solved in 2 secs!!

For the case of flowshops with three or more stages Jayanth discovered that unfortunately the procedure described above only provides an upper bound to the expected completion time. For this reason he has developed a rigorous branch and bound and method that works as follows. At the root node the completion time is computed with mean processing times which yields a lower bound of the expected completion time. Branching is then performed in the space of product sequences so that every time a given product is fixed, it is “exploded” into its discrete random states which are used to update the expected completion time. All the calculations involved in the branch and bound search involve the application of recursive algebraic formulas. A preliminary version of this tree search algorithm has been applied by Jayanth to problems with up to 8 products, 4 stages and 3 discrete states. He is currently investigating ways of improving the tree search so as to reduce the computations in the space of the states.

As indicated in the previous newsletter, another important extension that Jayanth has been investigating is the handling of continuous distribution functions. Rather than having to integrate analytically the corresponding pdfs he found that it is possible to use discretization schemes that provide excellent approximations, and in some cases exact answers. The idea relies on the fact that for univariate functions exact discrete approximations are possible for higher moments by the appropriate selection of discrete points that happen to correspond to roots of polynomials for Gaussian integration. Jayanth is testing of this idea on several examples. The important implication of this approximation scheme is that exactly the same approach can be used for both discrete and continuous probabilities.

Multiperiod Disjunctive Programming Algorithms

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

New Developments: *Lagrangean decomposition s for incorporating royalties in the oilfield planning problem*

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

Sarette first developed a general disjunctive formulation that considers as major discrete decisions selection of design (synthesis), operation of unit, and capacity expansion. This model involves embedded disjunctions that reflect the decisions of selection design -> operation -> capacity expansion. It also has as particular cases the "traditional" multiperiod design problem (i.e. no operation, capacity expansion), the capacity expansion planning problem (no 0-1 variables for operation), and the operational planning problem for a fixed design. Sarette developed a hybrid algorithm that relies on a bilevel decomposition

approach and a logic-based MINLP method for multiperiod operation. The bi-level decomposition consists of an upper level that is concerned only with the design variables and a lower level that is concerned with the operation and capacity expansion. The upper level problem requires the definition of a special problem that exhibits bounding properties, while the lower level problem is simply the original disjunctive program for a fixed design. Each level is solved with the logic-based MINLP method. This hybrid method proved to be very successful as it allowed the solution of process networks problems with up to 25 periods. In addition, Sarette applied her method to the multiperiod retrofit design of multiproduct batch plants. In the largest problem, a 4 product, 4 stage plant problem with 4 time periods, the MINLP with 832 0-1 variables, 769 continuous and 2422 constraints, was solved in 13,000 secs to optimality. DICOPT could not solve this problem.

Sarette has developed a nonlinear model for the offshore oil facilities planning problem. Ramesh Iyer in collaboration with Sriram Vasantharajan and Stan Cullick from Mobil Technology had used a piecewise linear approximation to model the change of pressure in the reservoirs and the corresponding cumulative flows. Using quadratic and exponential approximations, and using DICOPT, Sarette has shown that problem can be solved faster. However, the drawback is that due to nonconvexities the solutions are often suboptimal. Using ideas of global optimization, Sarette has used underestimators to increase the likelihood of finding the global optimum. Since the computing times may still be rather high, she has investigated a strategy that makes use of the bilevel decomposition and relies on aggregating time periods in the upper level problem. Sarette has developed a novel time-aggregation method that finds the optimal length of the time periods. Based on the idea of "matching" as close as possible the net present value, Sarette has developed a dynamic programming method for finding the optimal length of the time periods. Using this method Sarette was able to solve problem with up to 25 wells and 24 time periods. Her method requires about 20 minutes of computation compared to about 6 hours that are needed when DICOPT is used to directly solve the problem. A manuscript describing this work is enclosed.

Sarette has been recently concentrating in the case when royalties are included in the objective function of the oilfield problem, which currently only involves the net present value of investment and operating expenses. The handling of these royalties is quite complex because they are not given as explicit functions. Royalties are a result of complex rules that involve tax incentives for long term investment. These rules are normally given in terms of gross revenues and investments, which incur different percentages of royalties depending on the net earnings. Most optimization models in the past have ignored these royalties due to their complexity. For a variation of the oilfield problem I which the major decisions are involved in the selection of well platforms and their interconnection with pipelines, Sarette first developed both "big-M" formulations for mixed-integer programming, and disjunctive programming models. She showed several interesting results. Not including royalties in the objective function can lead to very different solutions even if heir effect appears to be small. Second, using big-M formulations the computation can be increased by one or two orders of magnitude compared to the case when royalties are not included! Sarette obtained reductions by several factors using the disjunctive model, but only in the smaller problems. In the larger problems there was no substantial difference as described in the enclosed paper in this newsletter.

Sarette has recently investigated a new a specialized algorithm based on Lagrangean decomposition for the problem described above. The basic idea behind Lagrangean decomposition is to exploit the structure of a model if it seems that very few variable link separate sets of constraints, by duplicating these variables such that each constraint set contains a different variable, and thus decomposing the model. In the case of oilfield infrastructure planning, this is especially appropriate, since each well platform has hundreds of constraints associated with it, and is only linked to other platforms through the pipelines. By duplicating the pipeline variables, and assigning one variable to each well platform, the model becomes completely decomposable over each platform. The constraints that link the platforms, i.e. the ones that sets the duplicate variables equal, are removed to facilitate decomposition of the model, and replaced with a penalty in the objective function. This penalty is the product of the deviation in the removed constraints, and the associated Lagrangean multipliers (hence the name "Lagrangean decomposition").

The largest problem Sarette solved consists of 16 well platforms, with a choice of 23 pipeline connections, to be solved over 15 years and the optimization model consists of 12696 constraints, 7633 continuous variables and 919 discrete variables. After decomposition, each subproblem consists of typically around

1500 constraints, 1000 continuous variables and 80 discrete variables. When attempting to solve only half this model in the full space, no solution could be found in more than 3 days, while with Sarette's proposed algorithm a good solution is found in just more than an hour. In one day of computing, a solution with a 5% increase in the NPV was found above the case without complex economic rules, translating into millions of dollars of savings.

Integration of Product Testing and Planning of Batch Manufacturing Facilities

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

Christos has started to work on this new research project that involves the development of an optimization model and solution method for the simultaneous testing for new product development and planning and design of batch plants. The specific problem which arises in agricultural chemicals and pharmaceuticals is as follows. Given is a time horizon over which a set of new products that have been discovered in research are to be tested for certification to meet FDA regulations. Costs, duration and probabilities of success of each test are known. Given are also existing batch manufacturing facilities, as well as potential plant configurations that may be used to manufacture the potential products. During that time horizon it is also possible that existing products may be withdrawn from manufacturing. The problem then consists in determining the schedule for testing of the products, as well as the selection of batch manufacturing facilities (existing or new) for their manufacturing in the event that the products pass all the tests. The objective is to maximize the expected net present value of the project. The reason this problem is significant in practice is that currently no systematic methods for deciding when to start preliminary design of the batch plants, nor of knowing whether it is best to use existing facilities t accommodate new products or building a new plant. Based on the previous continuous time model by Craig Schmidt for scheduling for new product development, and a discrete time linear model for flexible process networks by Norton, Christos has been able to integrate both models through a novel MILP model. The basic idea in this model is to define scenarios that may arise depending on the outcome of the tests for the products, and take advantage of the discrete times to define potential termination points for the testing on the products. Christos is in the process of testing this model on several problems.

Supply Chain Dynamics and Control

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

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

This is a joint project with Erik Ydstie in collaboration with Turaj Tahmassebi. from Unilever. The problem that Edgar has initially addressed is the one of determining the dynamic response of a supply chain to perturbations in the demand. The supply chain considered is one that consists of a manufacturing plant, warehouse, distribution center and retail center. The manufacturing plant can produce multiple products. In this supply chain there are material and information flows that go in opposing directions: the material flow from the plant to the retail center; the information flow from the retail center to the manufacturing plant in the form of orders. When disturbances occur in the demands at the retail level, there is often an amplification of the orders upstream due to the decentralized decisions made at each point of the of the supply chain. Therefore there is interest in determining the accumulation of inventories at each point of the supply chain. Edgar modeled with tanks the accumulation of material and the accumulation of order at each stage of the supply chain. Also, he postulated delivery rates for the materials as well as control laws for the decisions at each point of the supply chain. For the manufacturing plant a similar control law was postulated which in effect corresponds to a heuristic scheduling method. The dynamic simulation of this model corresponds mathematically to the solution of a hybrid system since discrete decisions are involved in terms of switching manufacturing to different products in the plant, and in terms of managing the inventory levels at each stage. Edgar was able to model the problem in Matlab and solve it using Signalflow. He was then able to analyze with different control laws (eg feedback based on set point for inventory levels) how closely the supply chain was able to track the demand of customers, as well as determining the dynamic response in the inventory levels. A paper describing this work is enclosed in this

newsletter. The next step of Edgar will be to incorporate optimization at the level of scheduling in the manufacturing plant, and as a global model for coordination all stages in the supply chain and provide the parameters of the control laws.

Software for MINLP Optimization in Design and Scheduling

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

New Developments: *DECAY and NETCHAIN interfaces*

Gabriela has taken over the work by Luisa. First she has continued the development of the new interface NETCHAIN, which deals with supply chain optimization for process networks with flexible processes which is based on the work of the visitor Jin -Kwang Bok from KAIST (a copy of that paper is enclosed). This interface is almost completed and is at the stages of testing the graphic output which is very extensive as it simulates material flows and inventories over a large number of time periods. Gabriela has also essentially completed the development of the new interface DECAY, which is based on the work by Vipul Jain for the cyclic scheduling of parallel furnaces that exhibit decay in the conversion due to coking. This interface automatically formulates the MINLP model for determining the optimal cycle time, assignment of feeds to furnaces, and number of subcycles for performing maintenance in the furnaces.

Zdravko Kravanja and Ignacio have recently received a US-Slovenia research collaboration grant. The objective of the work will be to further enhance and improve the code PROSYN-MINLP that currently runs on Windows-NT. This code will be reimplemented as the new code MIPSYN that makes direct use of the recent developments in disjunctive programming.

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

Synthesis:
SYNHEAT MINLP synthesis heat exchanger networks *(Yee)*
Also includes transshipment model for targeting *(Papoulias)*
STEAM MINLP Model for the synthesis of combined cycles for utility plants (Bruno)
Model includes correlations for steam, efficiencies and cost data
GLOBESEP Global NLP optimization for synthesis of separation networks and
single feed/mixed products *(Quesada)*

Batch design:
BATCHSPC MINLP and MILP models for multiproduct batch plants
single product campaigns *(Kocis, Voudouris)*
BATCHMPC MILP model for multiproduct batch plants
mixed-product campaigns *(Birewar, Voudouris)*
Scheduling:
PARALLEL MINLP continuous multiproduct scheduling on parallel lines
Features feasibility preanalysis *(Sahinidis)*
MULTISTAGE MINLP continuous multiproduct in multistage plants *(Pinto)*
CYCLE LP/MILP aggregate flowshop scheduling (cycle time/makespan)
Includes loop tracing algorithm *(Birewar)*
STBS MILP short term multistage scheduling *(Pinto, Bolio)*
CRUDEOIL MILP model for refinery scheduling *(Lee, Pinto)*
PRODEV MILP model for scheduling of tests in new product development *(Schmidt, Najimas)*

Planning:
PLANNER MILP multiperiod model for capacity expansion in process networks
(conventional and lot sizing model) *(Sahinidis, Norton)*

MULTISITE MILP model for planning the selection of processes and capacity expansion in different geographical location and accounting for transportation costs *(Turkay)*

GREENPLAN Bi-criterion MILP model for selection of processes that maximize the net present value and minimize toxicity *(Drabbant)*

Steinar Hauan's Group

Feasibility and Economics of Reactive Separation Systems

Students: Warren Hoffmaster (Ph.D. started Jan 2000)
Vikas Verma (Ph.D. started Jan 2000)

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

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

Using the theory of generalized difference points developed in collaboration with Art Westerberg's group, we are studying the feasibility (Warren) and economics (Vikas) of reactive separation processes. Specifically, Warren is preparing thermodynamic subroutines along with a module for bifurcation analysis in Matlab to address reactive and non-reactive pinch point curves as well as limiting conditions for sectional cascade profiles. Vikas has started work on collocation models for hybrid processes with simultaneous reaction and separation with the goal of an ASCEND implementation.

Microscale Process Synthesis

Student: Gogi Singh (Ph.D. started Jan 2000)

Gogi will work on adapting traditional systems approaches to fluid flow, chemical reactions and heat transfer to design and operation of microscale systems. The goal is to find the proper level of modeling detail of these units in order 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.

Initial work has been in numerical simulation of flow patterns in for various geometries representing standard "unit operations" in chip-based system such as channels, wells and valves. The next step will be to incorporate chemical reactions in order to investigate the effect of geometry on microscale mixing and thus efficiency of small scale reactors.

Flexible Synthesis of High-Value Products

Student: **Murni Ahmad (MSc started Jan 2000)**

Co-adviced by Todd Przybycien in biomedical engineering, Murni will work on optimal design and operation of pharmaceutical and biochemical processes. In addition to regulatory constraints imposed on the operation of actual equipment, modeling is further complicated by incomplete knowledge of the biological mechanisms involved and different assessment of time-to-market aspects compared to production of bulk chemicals. A key issue is to capture the economic interactions between efficiently designed processes in new equipment in light of procedural requirements for FDA approval.

Murni presently focuses on optimal scheduling of a reactive batch experiment with a two-stage chemical reaction limited by equilibrium where complete conversion must be guaranteed. She has also started a study on optimization of a protein separation system involving two-phase aqueous solutions.

Arthur Westerberg's Group

***n*-dim (*n*-dimensional Information Modeling)**

Coworkers: **Michael Collins (Staff programmer)**
Helen Granger, Graphics consultant
Suresh Konda, Software Engineering Institute Staff (Ph.D. - Business)
Eswaran Subrahmanian, EDRC Research Faculty (Ph.D. - Information Technology, Business School)

Student: **Russell Milliken (Ph.D., started August, 1995, completed May, 2000)**

BACKGROUND (skip to the PROGRESS section below if you are familiar with this project)

n-dim: The *n*-dim system is a computer environment to support the information management needs of a geographically distributed team where the team is carrying out a major activity such as the design of a new process or product. Our primary hypothesis for narrowing down what *n*-dim should be is that designers are continually creating models - not only of the artifact they are designing, but also of the design process (an activities model), of the organization, of the unofficial contacts they make in the organization, of the information they have gathered, etc. Therefore, we have created *n*-dim as a very general modeling environment, which allows people to store and interrelate information of all sorts, each on his/her local computer. In *n*-dim the building blocks for models are pointers at objects and labeled links. A labeled link connects two object pointers and implies a relationship between the two objects. It allows diverse objects such as drawings, memos and quantitative models, to be linked together to form other models. Overall the interlinked structure becomes a "web" that spans all the computers on which the group stores its objects.

n-dim stores models and object attributes in databases, making it possible to find objects by searching over their attributes and/or over the models in which they appear – e.g., over the structure imposed over that information. We are able to create models that act as shell scripts to launch external programs and to transfer information from the output of one external program into the input of another (to emphasize, the scripts and the wiring information are themselves *n*-dim models); we can model people and groups of people and will be able to use these models to define access control for the system; we can use these same models within an e-mail system. We are able to create modeling languages to help others create special types of models. The languages are themselves expressed as *n*-dim models.

The *n*-dim project completed a major project with a large international product manufacture to study and then improve information flows in a part of their company. This study resulted in our creating a prototype document management system designed together with their engineers. We have also completed a joint project with ABB in which we captured the data flow throughout the design of a product they produce. We

have participated in a multi-university/company project funded by DARPA to study how to make design support services available over the internet, providing the history capturing mechanisms for transactions taking place over the internet by the various participants.

LIRE': We revised the document management system mentioned above into a system we call LIRE' (LIving REpository), a system that the ICES community and others are now using to manage documents. LIRE' features web access so documents may be up- and down-loaded onto a computer from anywhere on the internet. All documents are retrieved in native form (e.g., as a Word - any pedigree, Framemaker, Excel, PowerPoint, a gif file). We have created a server, which can operate on another machine that will convert native form into a PDF version and a text version. These too are saved along with the native. The native version is there to support collaborative document creation. Users can create a version and upload it for storage in LIRE'. A collaborator anywhere on the internet can download the native and work on it. Saving it creates automatically a new version with the old kept in the background. The PDF version serves as a universal form that anyone can display. It also is the version that we will continually upgrade to new PDF versions as needed to guarantee future visibility. The text version allows us to carry out search over content. LIRE' also features a keyword web wherein keywords (a keyword in LIRE' is both a word and a definition) may be related through refinement, generalization and translation (German to English, for example). Thus one can find related documents by searching over keywords related to those specifically used in describing it. All documents may also be linked to other documents – e.g., with a "background" link. One can search over these links to find documents also. Finally, one can add annotations to any of the documents, providing a form of informal review. LIRE' also has access control mechanisms to control who can see and modify what. It is about to have a new more familiar look and feel to it for PC users. And it is about to have full notification service, whereby a user can ask to be notified if a particular document is altered in any of a number of specified ways.

Co-editor: As a part of his Ph.D., completed in May, 1998, Doug Cunningham produced a co-editor that allows end users to write operations in *n*-dim without being experts in Python or Java, the languages used for operations. It watches what one does in a sample session and develops a program to emulate it. What is particularly nice is the way the co-editor discovers relationships among the objects involved in the sample session. A subset of these relationships, while not stated nor necessarily evident to the user, is often the reason the person selects the particular combination of objects in the session. Thus the co-editor shows the user these relationships while asking him how to generalize the code it is writing. If the proof of a concept is in its usefulness, this one proves to be extremely useful. It is the way we now write most of the operations. It was in direct response to our hypothesis that support systems must allow the end user to participate in significant ways in the evolution of a support environment.

JDBC database compatibility: Russ Milliken implemented a new database interface to allow *n*-dim to tie to any JDBC compatible database. We currently use Oracle, which is available at CMU. A part of this interface is a very fast in core cache memory for all recent transactions that have speeded up database access significantly. It is possible to use only this cache with a file backup to mimic the existence of a database for small personal installations of *n*-dim.

PROGRESS

AWARE: a notification server: Russ Milliken has completed the coding, testing and installation of his AWARE system for handling notifications. It functions as an independent server and can be used by any number of applications. He tested it for use in multiple LIRE' and *n*-dim installations. The notification server is also its own customer. It can ask to be notified if any part of it is restarted after being down. Russ developed his design so the system can survive the failure and restarting of any part of it. It uses an existing 10,000 event/second single event server package called Elvin, a package that is available from a group in Australia. It was also designed to allow expansion of the system to virtually any size by allowing all of its components to be duplicated to spread the loads.

We describe very briefly here the typical use of this system.

1. Any new application program that starts first registers itself with the system. Registering involves telling the notification system about all the events this application program will report and the type of parameters that will be part of that report.

2. An application program can then express interest in any event type that the system knows it or some other application may report at some time in the future. This is called subscribing. The event may be simple or complex, rather like setting up a query for data from a database. It subscribes by calling a bit of client-side notification software that is installed on the computer on which it resides. The client-side software passes the subscription to any one of the notification servers to which it is attached, each of which will typically reside on a different computer. The notification server analyzes the subscription, accepting it if it is properly formulated. It then takes each individual event subscription embedded in the original subscription and subscribes to all Elvin servers to which it has access. This multiplicity of subscribing is not a problem as subscriptions happen only infrequently relative to events and only one of the Elvin servers will have the event reported to it (see the next item). Subscriptions can have elapse times associated with them, at which time they get dropped.

3. When an event happens, the application program reports it through its client-side code, which passes it to one of the notification servers to which it is attached. This notification server then passes it to one of the Elvin processes to which it is attached.

4. On receipt of an event, Elvin matches it with the subscriptions it has in hand. If there is a match, it triggers a call back to the notification server that sent it the subscription. This notification server then matches this event against any complex events on its stack. Ultimately the event leads to a call back to the application program that placed the original subscription. This final call back receives all the parameters associated with the event.

One use of this system is for the notification server to use itself to detect and recover from the failure of any of the components in it. For example, whenever one restarts a component within the notification system, the component can report this as an event, an event to which the notification server has itself subscribed. When it receives such a notification, it can take remedial action. For example, if it is a restart of an Elvin server, it can resend all the subscriptions to it that have not been cleared.

Another use is to establish a negotiation process for a person to "push" a notification onto someone else. As a user of LIRE', for example, I can ask to be notified if person 'X' or any one of the persons in a particular group posts an event that he wants me to receive a notification whenever he changes one of his documents. I can then choose whether or not to place this subscription -- i.e.; I can control who can send which notifications to me.

The first use of this notification server is with LIRE', our document management system. Russ designed all the events that LIRE' should report, selecting them to be at the level of "create a new document jacket," "store a new version," or "add a new folder." He then worked with Michael Collins and Helen Granger to get LIRE' attached to AWARE. LIRE' has a very nice interface now for someone to select which event he/she wishes to become aware have occurred. When one occurs, a moving banner crosses the LIRE' screen at the bottom if the recipient is using LIRE' and the recipient gets an automatic e-mail telling about the event. Russ provided this system to two general engineering design classes here at CMU to test how useful students would find it. Some of the students – not all – used notifications extensively in their group work.

Russ also worked on the development of an engineering change notification system on a project with Adtranz. We intend for his notification server to be an integral part of this system.

Russ finished his Ph.D. this last May. He will be working for a local start-up company here in Pittsburgh, starting in mid-July.

***n*-dim:** We are adding features to the *n*-dim environment.

Erika Fleckenstein (a senior Chemical Engineering student, who just graduated and who has done projects with our group since her sophomore year,) just developed, through "doing it," a general methodology to create a new application program using *n*-dim (she used the network model to define the data structures and the operations on those models to provide the behavior – see Doug Cunningham's contributions described above). Specifically she developed an IWEB application (to support suggesting and resolving issues) to illustrate the approach. Once she had an IWEB capability in *n*-dim, she used it as the specification for creating a java version, which she handcrafted. She then tied the java version back into *n*-dim so the exact same capability is still in *n*-dim except it is much faster. She developed a list of tools, which, if they existed, would have significantly reduced the time she took to carry out this project. The goal is to make this methodology available to end-users of *n*-dim – or at least almost available.

We are tying *n*-dim to LIRE' so when one is in LIRE' one will be able to click on a stored object and cause *n*-dim to start. In this manner we can get people at least to look at *n*-dim with no real effort expended on their part. When in *n*-dim, one will also have access to all the different types of objects that are in LIRE'. We expect this coupling will allow end users to augment the capabilities of LIRE' without the aid of a staff programmer, using the ideas of Erika's work above.

Process Synthesis Using Units with Integrated Functionality

Ph.D. student	**Jae Woo Lee (started August, 1997, finished May 2000)**
Collaborators	**Steinar Hauan**
	Ignacio Grossmann and Hector Yoemans
	Jeff Siirola (Eastman Chemicals Co.)

Background: Our goal for this project is to use and extend concepts available in composition space for designing processes. We would like to discover insights to allow a designer to know quickly when a combination of functions (e.g., reaction, mixing and separation) within a unit is beneficial for a design. Steinar Hauan, when visiting here while still a graduate student in 1997, discovered the existence of a **reaction difference point** in composition space. In the earlier Ph.D. work with Oliver Wahnschafft, we developed insights based on using difference points when carrying out extractive distillation. Our first efforts have been to merge these two ideas to see the implications for design.

An earlier publication based on the work presents the reaction difference point and how to represent movements in composition space based on adding vectors representing mixing, reaction and vapor/liquid separation. A second publication involves Amy Ciric. It arises from discussions that we all had (Lien, Hauan, Ciric and Westerberg) while here at CMU to combine ideas on reaction and extractive distillation. Both were a part of Steinar's Ph.D. thesis with Kristian at Trondheim, Norway. This second work looks at the movements possible in a (ternary) reactive extractive distillation column based on combining reactive and extractive difference points.

Jae Woo Lee joined this project in the late fall of 1997. First he took the course that Kristian taught on process synthesis – a course that emphasized distillation and reactive distillation. Jae, with input from Kristian, Steinar and Art, prepared "part II" of the second paper mentioned above. Jae realized the usefulness of creating a pseudo-feed point for a reactive distillation column that mixes the desired products. Then the movement from the actual feed to the pseudo feed must be accomplished by reaction. He found a **new lever rule** that involves the lengths of two different lines that allows him to place the column difference point when the reaction difference point is at infinity. These ideas allow him to produce possible design alternatives for such processes by sketching them in composition space.

Jae next determined **how to construct both McCabe-Thiele and Ponchon-Savarit diagrams** for binary distillation **that includes reaction** on the trays. Two reactions are possible for a binary mixture: (1) isomerization: B <===> A and (2) decomposition B <===> 2A. This work came from trying to extend the vector space in which straight line mixing occurs to include temperature and pressure effects. We examined using coordinates that reflected conserved quantities: material, energy and momentum. This worked as we found that temperature can be considered by using molar enthalpy as the spatial coordinate.

We can add pressure by considering molar momentum, but it seems to hold only for a trivial case, which makes it of less interest at present. Both diagrams are very easy to construct.

When one examines this diagram, one can readily "see" where to place reaction within a column by sketching. One does not need accurate simulations. Of interest was that, at least to us, the **placement of the reaction zone was counter-intuitive**. For example, if the product of the reaction is the light product, the reaction zone is best placed above the feed. We imagined it better to place it below as then the reactant would proceed down the column and react to form the light. However, it is better to place it above, which results in a smaller column and less reflux to accomplish the desired product purities. Similarly, if the reactant is the light, then it is better to put the reaction zone below the feed. This result seems to be the first to provide a rule of thumb about placement of reaction within a column.

Jae also found two isomers that form an azeotrope. Reaction in a column permits one to break the azeotrope. One can readily visualize the very nonintuitive result of having a portion of the column below the reaction zone increase the composition of the more volatile component as one goes down the column. The consequence from this is that temperature will decrease as one moves down the column. These ideas relate to the placement of difference points mentioned above. The intersection of the operating line with the 45 degree line on a McCabe-Thiele diagram is a difference point. We do not see how to expose these results with any of the previous work in the literature on reactive distillation. Indeed, we suspect this earlier work would not suggest one could **step past the azeotrope**.

Jae spent **two months at Eastman Chemicals** in the spring/early summer of 1999 working in the synthesis group run by Jeff Siirola. He returned with ideas on how to do the tray-by-tray stepping in a column graphically.

Jae developed as approach to finding the **reachable products** for a binary reactive distillation.

Progress: Jae extended these ideas to systems involving three and more species. He developed graphical methods to examine both the MTBE (treated as a 3 component system) and the ethyl acetate (treated as a four component system) reactive columns. He was able to establish graphically where one has to place reaction in these columns. He also developed a projection technique that allowed him to discover graphically and quantitatively the best value for the reflux ratio to use in the latter system, falling in the range given in the patent literature for this process. A first draft of a paper on this work is part of this newsletter.

Life Cycle Analysis with Structured Uncertainty for the Synthesis of Process Flowsheets

Ph.D. student: Lifei Cheng (started August 1998)

Background: Collaborating with Profs. Biegler and Grossmann on a DOE funded project, we are looking at developing a design methodology and supporting tools to study processes from a life cycle perspective.

This project started with John Clark. John's goal was to develop methods for the synthesis of future scenarios for a process. So rather than synthesizing processes, he proposes to synthesize scenarios. He anticipated where future technology might challenge a process. He explored the use of a so-called "free step" (originally proposed by Bill Johns and his student Romero in the 1977 and 1979). If one can have any step in the process for free, then by how much would the process and its economics change? If a step allows for significant improvement, then it becomes a candidate for assessing the possibility someone might figure out how to do it. Together this information will aid one to assess the possibility such a technological breakthrough could threaten the current design.

John Clark completed an MS degree on this project in the spring of 1999. In his thesis he looked at an economic objective to assess when a new process will threaten an existing one. He devised different types of free steps that could result from a breakthrough in technology. One is a magic separation step where one removes product from a reactor that is equilibrium limited, thus allowing the reactor to completely convert

the reactants. Having such a technology can dramatically alter the process design and its economics. To determine if a proposed technology breakthrough can be a threat, he synthesized a new process based on it. He then asked if this new process is viable when the current process only has to recover its operating expenses; essentially the existing process will write off its investment costs when threatened. For a breakthrough that can be a threat, one must then assess the probability the technology leads to a new process in five, ten, fifteen or twenty years. He proposed to calculate the expected value of the present worth over all the possible scenarios. The ratio of this expected value to the value if there is no risk gives one possible vulnerability index for a proposed design.

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

He then demonstrating that he can model events (using ideas that Vicente Rico-Ramirez developed early in his Ph.D. project) non-procedurally. He also demonstrated that he can model queues (e.g., an order can be added to a queue to be processed later), time delays, and so forth, in a non-procedural modeling system (yes, ASCEND). The conjecture is that this approach to developing these models will be very easy for a typical modeler, a conjecture we have yet to prove. It may be hard for a person steeped in the traditions of procedural modeling at first, however, as it will represent a very different way to think. The idea is that one simply says what has to be true and not the order in which things will happen. The truth can include events happening when something starts to boil, for example, and for the system to alter its modeling equations for times that follow when that happens. You are probably thinking about this procedurally while it is being described here. The trick is to think clearly and easily about it non-procedurally. When (not if) that becomes possible, then we can model both physical artifact and its operation in the same language. The solvers will not care which is which.

Progress: Lifei has found several articles in the business literature that considers business decision making based on stochastic models for the future. In one, the approach leads to a “dynamic programming” like algorithm for stating and then solving. In effect the problem statement is recursive. He is now investigating some example problems to assure that we understand this paper. We can see the need for some very interesting capabilities in a solver for such problems if we are to extend the capabilities of a system like ASCEND to set up and solve such problems.

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