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Final Report

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

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In this project we investigated methodologies for the synthesis and analysis of process flowsheets over a life-cycle in which there are significant technical and economic uncertainties, and in which investment, energy and waste management are major issues. Three Ph.D. students are involved in this research project (Lifei Cheng, Sarette Van den Heever, William Rooney). The major items that we addressed are the following:

1. Development of conceptual synthesis methodologies that will aid in the possible identification of potential new technologies and "breakthroughs" in process design. We developed a rigorous dynamic programming approach based on Markov decision processes (MDP) for solving a stochastic optimization problem that incorporates higher level design decisions and lower level production decisions. Using insights from this rigorous approach we are developing approximate methods to allow us to solve realistic problems.

2. Development of optimization models and tools for effectively solving multiperiod-multiscenario problems, with special emphasis on the application of oilfield planning problems. Major concerns are the development of techniques for problems that involve nonlinearities in the model with many time periods or scenarios, and complex economic objectives that result for the consideration of royalties, tariffs and taxes.

3. In the area of reactor network synthesis, we have developed a new math programming based algorithms for the systematic construction of attainable regions. In addition, we have modified the flexibility approach of Grossmann and coworkers to deal with uncertainty associated with nonlinear model parameters. This strategy incorporates <u>nonlinear</u> confidence regions into the uncertainty description in an efficient way and leads to a more realistic characterization of the impact of model uncertainty. We has also extended this to problems where uncertainty falls into two categories: one that is compensated by feedback and another that requires a robust design.

1. Synthesis of Uncertain Events

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

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

He then demonstrated that he can model events non-procedurally (using ideas that Vicente Rico-Ramirez developed here early in his Ph.D. project). 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 (ASCEND, see http://www.cs.cmu.edu/~ascend). The conjecture is that this approach to developing these models will be very easy for a typical modeler. 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. Using non-procedural modeling, we can model both a physical artifact and its operation in the same language and solve either or both with the same solvers.

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

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

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

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

Lifei (Cheng et al, 2002) developed a small problem involving only discrete decisions and states on which he tested the various approaches possible for solving. He used dynamic programming to solve from an end time backwards to the current time. He also showed how to expand the problem to all of its equations and solve as a large simultaneous problem. He argued that often one can partition a problem into a nonstationary first few years and then a stationary problem from then on. One can solve the stationary problem first and use its solution as a boundary condition for the non-stationary part. A stationary problem is often much easier to solve.

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

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

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

into the problem

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

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

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

Lifei is currently developing approaches to solve much larger multiobjective stochastic optimization problems. He has been reviewing an extensive literature on the solving of such problems for single objectives. Much of that literature involves solving through the use of scenarios and noting their bordered staircase structure. Lifei is also using multiple scenarios as the basis of his approach but is taking advantage initially of the structure by using procedural simulation models – namely, given some parameters, the starting point and the scenarios, simulate the problem behavior and determine the values for the multiple objectives for it. An outer optimization loop will adjust the parameters.

He is reducing the problem size dramatically by finding an "optimal" parameterized decision policy rather than the full set of optimal decisions at each instant in time. For example, one can choose to set the manufacturing level by controlling the level of inventory. If the inventory level drops below the value of a certain parameter, one can decide to manufacture another batch of material, where he finds the optimal value of that parameter to reflect his (stochastic) model of future behavior. He pre-generates the scenarios as a list of random numbers that each will use, moving the stochastic behavior outside the optimization loop. The newspaper reordering problem is a simple problem for which one can prove this type of feedback control is equivalent to the stochastic optimal control solution. Lifei is not expecting to be able to prove this equivalence for his problems as they are very highly nonlinear. Such simple problems suggest the structure that one might use for the policies one will use. Finally, he is seeking efficient methods to allow him to stop looking for improved solutions by adding more structure and thus more parameters to define the control policy.

Related to collaboration, a theme of this proposal, we [Milliken, 2000] implemented the notification server, AWARE, for supporting collaborative design and implemented and extensively tested it within LIRE', our web-based document management system. Students in several of our classes use LIRE' in supporting their design projects. The event and notification capability of AWARE allows the timely exchange of information among collaborating designers. By using itself AWARE is also very robust and can recover from events such as computer outages.

Finally, with John Siirola and Steinar Hauan (Siirola et al, 2002), we have been studying the impact of collaboration on the effectiveness of agent-based systems to solve very large problems, such as that being posed by Lifei Cheng. Siirola's work is developing measures to assess this collaboration. Examples show its impact is extremely significant.

2. Multiperiod-Multiscenario Optimization Techniques

This part of the project dealt with the optimization of process systems that operate under different conditions in a sequence of time periods. Examples include plants that deal with seasonal demands, or oilfield systems whose production and mix changes over a long time horizon. We have focused our work in the modeling and solution of these planning and design problems using as a basis disjunctive programming. The major focus of application has been in the design and optimization of oilfield planning problems. In the initial part of our work we 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, and capacity expansion. We developed a hybrid algorithm that relies on a bilevel decomposition approach and a logic-based MINLP method for multiperiod operation. This algorithm proved to be successful in the solution of process networks problems with 25 periods, and to the retrofit design of multiproduct batch plants with 10 time periods.

Our largest effort was involved in developing large-scale nonlinear optimization models for the offshore oil facilities planning problem. The first problem we considered consists in selecting the location and number of production and well platforms, as well as the schedule and identity of the wells to be drilled. For this problem the major challenges were the handling of large number of discrete variables, as well as the nonlinear models for pressure in the reservoirs and the corresponding cumulative flows. We developed a strategy that makes use of the bilevel decomposition and a novel time-aggregation algorithm. Using this method we were able to solve a problem with up to 25 wells and 24 time periods in about 20 minutes of computation compared to about 6 hours that are needed with the commercial MINLP solver DICOPT. More importantly the optimal solution yielded $12 million savings in net present value compared to a common heuristic procedure.

The second problem is the one in which we do not consider decisions on the drilling of wells, but we instead consider interconnections among the well platforms, as well as complex economic objectives that include royalties and tariffs. The handling of these economic terms is quite complex because they are given by complex rules that involve tax incentives for long term investment. These rules are normally given in terms of gross revenues and investments, which incur different percentages of royalties depending on the net earnings. Most optimization models in the past have ignored these royalties due to their complexity since their relaxations are very poor and the size of the problems is greatly increased. We were able to develop a Lagrangean decomposition technique that decomposes the problem into well optimization subproblems. Using this technique we were able to solve problems with up 16 well platforms, with a choice of 23 pipeline connections, to be solved over 15 years and the optimization model consists of 12696 constraints, 7633 continuous variables and 919 discrete variables. When attempting to solve only half this model in the full space, no solution could be found in more than 3 days, while with our proposed Lagrangian decomposition algorithm the optimal solution was found in about 33 hours, yielding a 5.7% increase in the NPV compared to the case without complex economic rules ($64 million improvement).

In the last part of this work we addressed the problem of hydrogen supply pipelines in collaboration with Air Products. The problem is the one in which a set of production plants for hydrogen is given, as well as several supply points in a pipeline that connects sources and destinations. Given a number of time periods with forecasts for demand the problem consists of determining the level of operation at each plant (e.g. which compressors to operate), as well as the policy for storing hydrogen in the pipeline through manipulations of the pressure. We developed a planning and a scheduling model, in which the planning model is concerned with determining the production targets in each plant, and the scheduling model the detailed delivery of hydrogen to each destination point. We used a rolling horizon strategy in which the planning model is solved successively with one period of the scheduling model. Since the planning model can become quite large, and represents the bottleneck in the rolling horizon, we developed a Lagrangean decomposition scheme that proved to be very successful. For instance, in a problem with 14 time periods the full space MINLP could not be solved within 10 hours, whereas the proposed decomposition method required only of the order of 20 minutes.

3. Uncertainty in Nonlinear, Reactive Systems

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 work in this area deals 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; these also build on our related research in development of simultaneous optimization strategies using 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 this project, 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. This work was led by William Rooney, who obtained his PhD in April, 2001. In addition, we have interacted heavily with Prof. Glasser's group at the University of Witwatersrand. In particular, Brendon Hausberger visited with us in Fall of 1999 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 is listed below. This visit led to prototype concepts for algorithmic generation of attainable regions. Shehzaad Kauchali continued this work as a visitor in our group in 2000-2001. In particular, in the area of reactor network synthesis, we have developed a new linear programming based algorithm for the construction of attainable regions.

In addition, we developed a framework to assess the design of reactor networks with uncertain kinetic and process parameters. This approach incorporates joint confidence regions obtained from experimental data within the reactor design problem as well as other process problems. Use of these regions leads to an approach related to flexibility analysis with some additional structure that can be exploited for efficiency. This approach leads to a multiperiod formulation with additional feasibility tests and 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. We have also refined this approach to deal with nonlinear confidence regions. While these are more difficult to generate, especially for larger problems, the confidence regions can be significantly different than for linear models and their impact of robust designs can also be quite different. We have developed a number of examples that illustrate this difference.

Moreover, we have considered more detailed approaches to uncertainty. Here we distinguish between unknown information due to process variability and uncertainties due to a lack of adequate knowledge of the process model. In the former case, control variables can be used to compensate for the variability, especially if these can be measured in a feedforward sense. In the latter case, one needs to develop a robust design that can accommodate all of the uncertainties of the process model. In an actual design application we will generally have both types and here the flexibility analysis becomes more complicated. We developed strategies that deal with both types of these uncertainties in a flexibility framework. To solve problems of this type we have also applied constraint aggregation strategies for the flexibility analysis. In an actual design application we will generally have both types and here the flexibility analysis becomes more complicated. We developed strategies that deal with both types of these uncertainties in a flexibility framework. To solve problems of this type we have applied constraint aggregation strategies for the flexibility analysis. Results on two process case studies show that the performance of these processes lies in between a conservative design (where control variables cannot compensate for variability) and an optimistic design (where control variables are allowed to compensate for all types of uncertainty). We believe that this leads to more realistic characterizations and designs with unknown information.

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