DOE/ER-14875-1

Final Report

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

L.T. Biegler, I.E. Grossmann and A.W. Westerberg

Department of Chemical Engineering

Carnegie Mellon University

Grant DE-FG02-98ER14875

July 2002

DOE Patent Clearance Granted

M. P. Dvorscak

2.6.03
Date

Mark P Dvorscak

501 252-2343

E-mail: mark.dvorscak@ch.doe.gov

Office of Intellectual Property Law

DOE Chicago Operations Office

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 (Lifeng 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 nonlinear confidence regions into the uncertainty description in an efficient way and leads to a more realistic characterization of the impact of model uncertainty. We have 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