1987

Advances in computer aided design

Lorenz T. Biegler
Carnegie Mellon University

Carnegie Mellon University.Engineering Design Research Center.

Advances In Computer Aided Design

by

L. Biegler

EDRC-06-38-87

ADVANCES IN COMPUTER AIDED DESIGN

L. T. Biegler, Department of Chemical Engineering, Carnegie-Mellon University, Pittsburgh, USA

Current research in Computer Aided Process Design can be classified into three basic tasks: analysis, synthesis and evaluation. This paper reviews improved methods for these tasks from a quantitative perspective. Specifically examples will be given in all three areas on applications of operations research, numerical analysis and mathematical programming to solve chemical process problems. To provide a flavor for this research the paper briefly outlines strategies for flowsheeting and continues with flowsheet optimization. Next process synthesis is introduced and the specific example of heat integration is described. A description of the quantification of process operability for evaluation is given. Finally, some future directions are defined and studies are cited that support these directions.

Introduction

Computer Aided Process Design (CAPD) has been an active research area in chemical engineering for the past thirty years. New developments are given wide exposure at semi-annual AIChE meetings and at least two or three international conferences are held each year that are devoted to some aspect of CAPD. Consequently, a complete description of recent activities in this area is clearly beyond the scope of this brief survey paper. For an introduction to this area, Seader (1985) gives an interesting survey of CAPD from a historical perspective. More detailed surveys of particular aspects of this field can be found in the two Foundations of Computer Aided Process Design proceedings (Mah and Seider (1980)) and Westerberg and Chien (1983)) as well as in the AIChE and Computers and Chemical Engineering journals.

Instead, this paper will focus on providing a flavor of the tasks and problems encountered in process design as well as some recent results in tackling these problems. In chemical and process engineering most tasks involving computer aided design can be classified under three general categories:

Analysis tasks - providing a description of process behavior. Often this task involves considering "what-if" situations.

Synthesis tasks - finding good solutions to open-ended design problems that have many alternatives, each of which may require an analysis task.

Evaluation tasks - finding a measure of how good a given design is for comparison with other designs.

Analysis tasks in chemical engineering typically require the solution of algebraic or differential equations in order to model or simulate a process. On the other hand, logical analyses of networks can be made for fault detection as well as qualitative description of a process (Lu and Motard (1985), Umeda (1987) and Andow (1985)). In the next section a case study will be presented that illustrates the use of flowsheet simulators in order to describe steady-state behavior.

Synthesis tasks for chemical processes deal with open-ended or poorly defined design problems where general goals are stated, many alternatives need to be considered and some search procedure is required in order to find a "good" if not optimal solution. A comprehensive introduction and review of this area can be found in Nishida et al (1981). Issues related to process synthesis involve compact and rich representations of alternatives, and generation of efficient search strategies for selection among these alternatives. In the third section of this paper the synthesis of heat exchange networks will be examined as an example of this task.

Evaluation tasks are often quite simple and are frequently embedded within analysis or synthesis tasks. Examples of these are the evaluation of profit, capital or operating cost, energy consumption, etc. However, many objectives are harder to evaluate rigorously although they are often just as important in ensuring well-designed processes. Among these objectives are safety, reliability, and operability. Although hard to quantify, recent developments in defining these objectives have led to effective evaluation procedures for these more difficult objectives. In the fourth section of this paper an outline of operability (or flexibility) analysis will be presented.

It should be emphasized that strategies to solve these design problems encompass a spectrum from heuristic and qualitative approaches to algorithmic and quantitative methods. The companion paper by Dr. Umeda emphasizes the former approaches and gives a broad summary of recent work in artificial intelligence and expert systems. This paper considers recent advances in computer aided design from a quantitative perspective. In particular, it emphasizes applications of concepts in applied mathematics dealing with numerical analysis, operations research and mathematical programming. In the following sections a few process examples illustrate how analysis, synthesis and evaluation tasks are tackled. The final section summarizes this approach and outlines some directions for future research.

Analysis for Computer Aided Process Design

By far, the analysis task is the one most often encountered task in process design. Moreover, a complete survey of this area is beyond the scope of this paper. Instead, to provide a flavor for this task it is useful to consider the steady-state simulation of chemical processes. Process simulation or flowsheeting can be described simply as the solution of a set of algebraic equations,

$$f(x) = 0.$$

These equations include:

- mass and energy balances for process streams
- unit operations equations for equipment sizing and prediction of component flows, pressures and temperatures
- cost equations for process economics
- physical property equations for calculating vapor-liquid equilibria, specific enthalpies, densities and other thermodynamic and transport properties

Taken together, these equations frequently number in the tens of thousands. To solve this set of equations, two simulation modes have developed over the past 25 years. The modular mode is by far the most common one and is virtually the only mode used in industry (see Motard et al (1975), Biegler (1984a)). Here all equations relating to a particular unit operation (e.g. separation, pumping) are solved for outlet streams and capacities once input streams and parameters are specified. The calculation order follows more or less the flow of material in the process with iterations required for unknown streams in process recycle loops. The advantage of this strategy is that simulations of large processes can be made very easily with general purpose modules.

In the equation oriented mode (see the review by Perkins (1983)), all equations are grouped together and a calculation strategy is found based on the structure of the equations. Here one has a great deal of flexibility in developing a calculation order and more efficient simulations can be made with this mode. However, equation oriented simulators are much more difficult to construct and, consequently, they have been slower to develop.

Consider now the task of "analyzing" what the optimum conditions should be for a given flowsheet. Here continuous parameters represent degrees of freedom in the process (e.g. feed flows, temperatures, pressures) and some objective is minimized subject to process and product (inequality or equality) constraints. Mathematically this problem can stated as:

$$Min<b(x)$$

$$s.t.\ g(x) \leq 0$$

$$h(x)=0$$

For process optimization with large scale simulation models a standard approach is to treat the simulation as a black box and to solve the flowsheet for different parameter values. On equation oriented simulators, this approach is usually efficient and successful since all equations, variables and, frequently, partial derivatives can be accessed by the optimization algorithm and the calculation order can be tailored to the optimization. For modular simulations, however, the black box approach can be especially expensive because recycle loop convergence, the slowest part of the simulation, must be done repeatedly for base point and for derivative evaluation (Biegler and Hughes(1982)).

Recently, optimization algorithms have been developed that allow the simultaneous solution of the simulation and optimization problem. Because recycle convergence can be handled this way, this approach is especially beneficial for the modular simulation mode. Moreover, simultaneous solution strategies based on Successive Quadratic Programming (SQP) (Han (1977), Powell (1977)) are quite effective in solving optimization problems for flowsheets with complicated and difficult recycle loops.

Consider, for example, the flowsheet for an ammonia process in Fig. 1 (Lang and Biegler (1987)). Here nitrogen and hydrogen are mixed, reacted at high temperature and pressure and the resulting ammonia product is removed by multistep flash separation. The optimization problem along with eight decision parameters or variables are shown in the figure and more specific information about the optimization problem and its solution is given in Table 1. The before tax profit, starting from an unconverged point, is improved from 20.66 to 24.93 million dollars/yr using a simultaneous solution and optimization strategy. For this process a conventional simulation of this process at the base point is time-consuming. However, the effort for process optimization requires only slightly more than two simulation time equivalents (139 CPU seconds on a VAX 8650) and is therefore cost effective.

Synthesis for Computer Aided Design

Briefly stated, the synthesis problem can be defined as designing the "best" process that satisfies given objectives from given specifications. This problem is frequently open-ended, not well-defined and many alternatives exist for its solution. To find reasonable solutions, the appropriate representation of the synthesis problem and an efficient way to search among alternative designs are particularly important. Consequently, the synthesis task frequently requires some level of analysis and evaluation to screen alternative designs.

Because of the open-ended nature of the problem, most of the progress in process synthesis has occurred with homogeneous process subsystems. For example, relatively efficient synthesis strategies exist for heat exchanger networks (Linnhoff, et al (1982), Floudas, Ciric and Grossmann (1985)), distillation column separation synthesis (Andrecovich and Westerberg (1985)), evaporation trains (Westerberg and Hillenbrand (1985)) and refrigeration systems (Shelton and Grossmann (1986). As expected, these synthesis strategies also span the continuum of heuristic to algorithmic approaches. In fact, heuristic approaches are often are very effective on problems that elude quantitative descriptions. Some synthesis techniques can also be aided by the use of simple targets or bounds (Douglas (1987)). Here, without actually constructing the final design, one can calculate a priori a bound that characterizes a good solution. The greatest success of targetting has been in the design of heat exchanger networks (Linnhoff et al (1982)). Using temperature-enthalpy curves that describe heat flows for the entire process, one can predict the maximum energy recovery for any given heat exchanger network dealing with that process. Consequently, the designer has an ideal solution to shoot for in building his network.

Papoulias and Grossmann (1983) have shown that this targetting procedure can be expressed as a linear program and can be generalized to multiple utilities and systems where exchanges of heat between certain streams need to be prohibited (for reasons of safety, location, etc.). Moreover, once the targets are known, matching the process streams for heat exchange can be formulated as a mixed integer linear program (MILP). Here continuous variables are used for the flow of heat throughout the process while discrete variables (0-1 decisions) are used to predict matches between process streams. Finally, since stream matches can lead to complicated networks involving bypasses or recycles, a general superstructure can be constructed with stream matches known, and the final heat exchange network can be found from the solution of a nonlinear optimization problem. Floudas et al (1985) have incorporated this fully automatic procedure for network generation into the MAGNETS program. In this way a difficult synthesis problem with many alternatives has been largely reduced to an algorithmic procedure. For example, Fig. 2 shows the heat exchange network for the ammonia process in Fig. 1. Here the profit is further increased from $ 24.93 million/yr to $ 26.91 million/yr as a result of energy savings.

Similar math programming concepts have been applied to synthesis of separation systems, integrated refrigeration cycles, and chemical reactor networks (Achenie and Biegler (1986)). However, many synthesis problems remain difficult to solve. Still largely unsolved, is the systematic synthesis of total process flowsheets (see Nishida et al (1981)). These involve complicated nonlinear relationships among process variables. Moreover, a rich enough superstructure of alternatives needs to be present in order to cover this problem sufficiently. Many interesting aspects of the total synthesis problem have been discussed in the early synthesis literature. More recently, progress toward the systematic solution of this problem has been made through devetopment of efficient mixed integer nonlinear programming strategies (Duran and Grossmann (1986a), Kocis and Grossmann (1987)).

Finally, a tot of industrial interest and activity is also focussed on the retrofit of process systems. Here the synthesis problem needs to address how existing equipment can be used in a new design. This additional requirement actually leads to many more design alternatives. Relatively little work has been done in retrofit synthesis and almost all studies have appeared in the past few years. A very recent survey of this area can be found in Grossmann, Westerberg and Biegler (1987).

Evaluation for Computer Aided Design

As seen in the examples above, process evaluation is often part of the analysis and synthesis process. Frequently the objectives are based on production, consumption or other economic factors that are readily quantified. More recently, it has been important to evaluate a process for less well-defined objectives such as process operability (Grossmann and Morari (1983)), reliability (Henley and Kumamoto (1985)) and safety (Andow and Galluzzo (1987)). These objectives have become increasingly important in the process industries with increasing competition, and the operation of more complex process under tighter operating specifications.

In the past, objectives such as safety and operability have been handled on a case by case basis with no systematic approaches procedures for general chemical processes. As expected, new safety guidelines were often motivated by posthumous examinations of accidents. More recently, non-numerical methods based on network and tree diagrams have been useful for predicting process faults and guiding the design of fault tolerant plants (Himmelblau (1978)). These concepts also lend themselves well to the construction of expert systems. Currently, the diagnosis of faults seems to be a very fruitful application of these tools (Andow (1985)).

In dealing with process operability much work has been done by using quantitative tools based on operations research and math programming. In the past, process design under uncertainty has been approached from a probabilistic perspective (Johns et al (1978), Malik and Hughes (1979)). Here uncertain external inputs, such as feed streams or ambient conditions, were generated by sampling probability distributions and the resulting optimization problem was further complicated. Several studies have dealt with this problem but all of them seem to suffer from large computational expense.

Instead, one can quantify a process' ability to operate under uncertainty by applying the concept of a *flexibility index* (Swaney and Grossmann (1985), Floudas and Grossmann (1987)). With an objective like this, one can evaluate profitability or energy conservation and trade these off against flexibility. As devetoped by Grossmann and coworkers, calculation of flexibility index involves finding the largest hypercube about the nominal point for which feasible operation can be tolerated.

Consider a quantitative model of the feasible region, i.e.

$$f_j(d,\theta,u) \leq 0 \quad j=1,\dots m$$

where 0 are the uncertain parameters in some region, d are the design variables (e.g. equipment sizes) and u are control or manipulated process variables (e.g. flowrates, pressures). The objective here is to find the limits to the uncertain parameters 0 where *for all* values of 6 within these limits *there exist some* u such that all m constraints are satisfied. Stated mathematically, calculation of a flexibility index F is given by the following math programming problem:

F = max§

sJ. $\max_{e} \min_{u} \max_{j} f_{\%}$ *(dfiji)* £ 0

$$\theta^N - \delta\Delta\theta \leq \theta \leq \theta^N + \delta\Delta\theta$$

Note that a flexibility index of unity implies that the entire region of uncertain parameters is feasible. For a flexibility index of zero, only the nominal values of uncertain parameters alone are feasible and for negative F no point is feasible. The geometric effect of the flexibility evaluation can be seen in Fig. 3. Here under certain convexity assumptions on f it can be shown that the expanding hypercube is limited at one or more of its vertex points. Swaney and Grossmann (1985) proposed an efficient algorithm to handle problems satisfying these assumptions. More recently, Floudas and Grossmann (1987) reformulated this problem as a mixed integer program that handles more general cases. However, except for problems with linear constraints, the mixed integer formulation is harder to solve. A successful application of this evaluation approach has been applied to the synthesis of flexible heat exchanger networks. Using the synthesis techniques mentioned above for the MAGNETS program, a network is constructed and evaluated for flexibility. For an F value too low, the parameters for the constraining vertex (see Fig. 3) are incorporated into a new network design and the procedure begins again.

The results of this analysis allow the designer to quantify a number of objectives in a given design and thus lead to consideration of trade-offs. Several other objectives can also be quantified through math programming formulations. Among these are the controllability of a process i.e. how quickly a process responds to handle external disturbances, the robustness of a controller design (Palazoglu and Arkun (1985), Wong and Perkins (1985)), and the toxicity of a process (Grossmann, Drabbant and Jain (1982)). Computation of these indices frequently adds another dimension to evaluation of new processes and thus leads to safer, and ultimately more economically efficient designs.

Conclusions

Recent advances in computer aided process design have been reviewed from a quantitative perspective. Here examples have been cited for analysis, synthesis and evaluation tasks, since most design activities can be classified under these three tasks. Here operations research and mathematical programming concepts which have led to significant advances in this field have been emphasized.

With advances in computer hardware and in the development of numerical algorithms, application of these quantitative tools is expected to increase and extend to much larger process systems. Currently, efforts are being focussed on solving larger nonlinear optimization problems for process flowsheets (see Locke et al (1983)). Also dynamic simulators are becoming better developed in order to describe process behavior for startup and upsets and to evaluate control algorithms (Aylott, Ponton and Lott (1985), Hillestad and Hertzberg, 1987). Successful applications of optimization to dynamic systems have been already been made (Biegler (1984b), Cuthrell and Biegler (1987)) and are expected to increase as larger optimization problems can be solved.

The seventies have seen a lot of research in the area of heat exchanger network synthesis that was spurred by the oil crisis. Now industries' needs have shifted and current synthesis activities are very much concerned with retrofit issues and consideration of total process systems. Here several heuristic approaches have been proposed and applied successfully (Douglas (1987), Lu and Motard (1985)). However, many interactions among subprocess systems need to be described in quantitative ways that often require computationally expensive models. Two recent studies address this issue for energy integration and retrofit design. Here rigorous flowsheet models are coupled with a flowsheet optimizer. In the first study (Lang et al (1987)), energy targeting constraints mentioned above and formulated by Duran and Grossmann (1986b) are included in the optimization problem. These targetting constraints allow for all heat integratton altematives for the process and lead to the optimal balance between raw material, capital, and utility costs. In the second study (Harsh (1987)) a mixed integer nonlinear programming strategy is coupled to the flowsheet optimizer and discrete process retrofit conditions can be made and evaluated with rigorous process models. Both of these studies indicate that a framework with rigorous models and optimization capabilities can be used for a wide variety of design tasks.

Finally, several objectives that could not be quantified except in case studies can now be formulated as optimization problems. Here the operability or flexibility of a process was considered as a novel math programming formulation. Future work will consider the incorporation of these objectives into complex flowsheet models for the routine evaluation of a process' flexibility as well as its economics. Also work is continuing on incorporating probability distributions into this kind of evaluation.

To complement exciting new tools based on object oriented and other novel programming concepts, the manipulation of rules and heuristics and the use of logic based non-numerical computing, much interest is being generated by optimization based design tools. In the future much work needs to be done in applying these tools to larger and more complicated problems.

References

Achenie, L and L.T. Biegler, "Algorithmic Synthesis of Chemical Reactor Networks Using Mathematical Programming,* I&EC Fund., 25, p. 621, (1986)

Andow, P.K., "Fault Diagnosis Using Intelligent Knowledge Based Systems", PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 145, (1985)

Andow, P.K. and M. Galluzzo, "Process Plant Safety and Artificial Intelligence", CEF '87 Proceedings, EFCE No. 349, p. 845 (1987)

Andrecovich, M.J. and A.W. Westerberg, "A Simple Synthesis Method Based on Utility Bounding for Heat Integrated Distillation Sequences", AIChE J., 31, pp. 363-375 (1985)

Aytott, M.R., J.W. Ponton, and D.H. Lott, "Development of a Dynamic Flowsheeting Program", PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 55, (1985) Biegler, L.T., "Simultaneous Modular Simulation and Optimization", in Foundations of Computer Aided Process Design - II, p. 369 Westerterg and Chien (eds.), CACHE Committee, (1984a)

Biegler, L.T., "Solution of Dynamic Optimization Problems by Successive Quadratic Programming and Orthogonal Collocation," Comp. and Chem. Engr., 8, p. 243, (1984b)

Biegler, L.T. and R.R. Hughes, Unfeasible Path Optimization of Sequential Modular Simulators" AIChE J., 28,6, p. 994 (1982)

Cuthrell, J.E. and L.T. Biegler, "On the Optimization of Differential-Algebraic Process Systems", AIChE J., to appear, (1987)

Douglas, J. M., *Conceptual Design of Chemical Processes,* McGraw-Hill, to appear (1987)

Duran, M. A. and I. E. Grossmann, "A Mixed Integer Nonlinear Programming Algorithm for Process Systems Synthesis", AIChE J, 32,592 (1986a).

Duran, M. A. and I. E. Grossmann, "Simultaneous Optimization and Heat Integration of Chemical Processes" AIChE J, 32,123 (1986b).

Floudas, C.A., A.R. Ciric, and I.E. Grossmann, "Automatic Synthesis of Optimum Heat Exchanger Network Configurations", AIChE J, 32,2, p. 276, (1986)

Grossmann, I.E., Drabbant, R. and R.K. Jain, "Incorporating Toxicology in the Synthesis of Industrial Chemical Complexes," Chem. Eng. Comm., 17, p. 151 (1982)

Grossmann, I.E. and C.A. Floudas, "Active Constraint Strategy for Flexibility Analysis in Chemical Process Design", Engineering Design Research Center, Report EDRC-06-07-86, Carnegie-Mellon University (1986) (Also to appear in Comp. Chem. Eng., 1987).

Grossmann, I.E. and M. Morari, "Operability, Resiliency and Flexibility: Process Design Objectives for a Changing World", Proceedings 2nd. Int. Conf. on Foundations of Computer-

Aided Process Design (Eds. A.W. Westerberg and H.H. Chien), p. 931 (1984).

Grossmann, I.E., A.W. Westerberg and L.T. Biegler, "Retrofit Design of Processes," paper presented at FOCAPO-87, Park City, Utah, July, 1987.

Han, S-P, "A Globally Convergent Method for Nonlinear Programming", J. Opt. Theo. and Appl.,22,3,p.297(1977)

Harsh, M.G., M.S. Thesis, Chemical Engineering Dept., Carnegie-Mellon Univ., (1987)

Henley, E.J. and K. Kumamoto, "Designing for Reliability and Safety Control", PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 651, (1985)

Hillestad, M. and T. Hertzberg, "Convergence and Stability of the Sequential Modular Approach to Dynamic Process Simulation," CEF '87 Proceedings, EFCE No. 349, p. 617 (1987)

Himmelblau, D.M., "Fault Detection and Diagnosis in Chemical and Petrochemical Processes," Elsevier, Amsterdam (1978)

Johns, W.R., G. Marketos and D.W.T. Rippin, "The Optimal Design of Chemical Plant to Meet Time-Varying Demands in the Presence of Technical and Commercial Uncertainty," Trans. I. Chem. E., 56, p. 249 (1978)

Kocis, G.R. and I.E. Grossmann, "Relaxation Strategy for the Structural Optimization of Process Flowsheets," I&EC Res., to appear, (1987)

Lang, Y-D and LT. Biegler, "A Uhified Algorithm for Flowsheet Optimization", Comp. and Chem. Engr., H, 2, p. 143 (1987)

Lang, Y-D, L.T. Biegler and I.E. Grossmann, "Simultaneous Optimization and Heat Integration with Process Simulators", Comp. and Chem. Engr., to appear (1987)

Linnhoff, B. et al, "User Guide on Process Integratton for the Efficient Use of Energy", I. Chem. Eng, (1982)

Locke, M.H., R.Edahl and A.W. Westerberg, "An Improved Successive Quadratic Programming Optimization Algorithm for Engineering Design Problems", AIChE J., 29, 5, p. 871,(1983)

Lu, M.D. and R.L Motard, "An Expert System for Computer Aided Flowsheet Synthesis" PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 517, (1985)

Mah, R.S.H. and W.D. Seider (eds.), Foundations of Computer Aided Process Design, Engineering Foundation, (1980)

Malik, R.J. and R.R. Hughes, "Optimal Design of Flexible Chemical Processes," Comp. and Chem. Eng., 3, p. 474 (1979)

Motard, R.L, M. Shacham and E.M. Rosen, "Steady State Process Simulation", AIChE J., 21,3, p. 417 (1975)

Nishida, N., G. Stephanopoutos and A.W. Westerberg, "A Review of Process Synthesis", AIChE J., 27, p. 321 (1981)

Palazoglu, A. and Y. Arkun, "Studies on the Design of Robust Chemical Plants", PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 457, (1985)

Papoulias, S.A. and I.E. Grossmann, "Structural Optimization in Process Synthesis II -Heat Recovery Networks", Comp and Chem Eng., 7, p. 707 (1983)

Perkins, J.D., "Equation Oriented Process Flowsheeting", in Foundations of Computer Aided Process Design - II, Westerberg and Chien (eds.), CACHE Committee, (1984)

Powell, M.J.D., "A Fast Algorithm for Nonlinearly Constrained Optimization Calculations", Dundee Conf. on Num. Analysis (1977)

Seader, J.D., "Computer Modeling of Chemical Processes," AIChE Monograph Series, §1, 15(1985)

Shelton, M.R. and I.E. Grossmann, "Optimal Synthesis of Integrated Refrigeration Systems," Comp. & Chem. Eng., 10,5, p. 445 (1986)

Swaney, R.E. and I.E. Grossmann, "An Index for Operational Flexibility in Chemical Process Design", AIChE J.f 31,4, p. 621 (1985)

Umeda, T., "Advances in Computer Aided Design," this conference

Westerberg, A.W. and H. C. Chien (eds.), Foundations of Computer Aided Process Design - II, CACHE Committee, (1984)

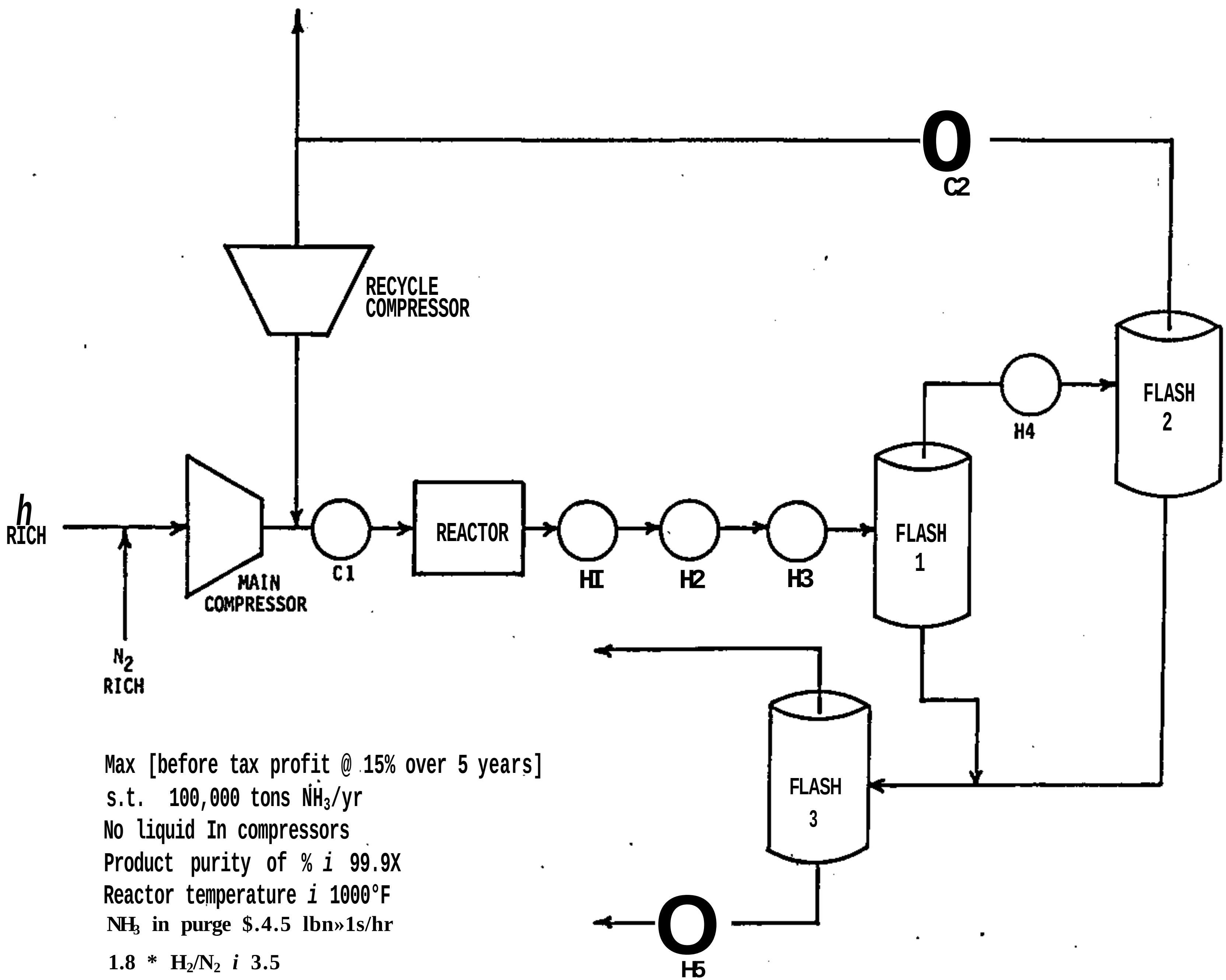
Westerberg, A.W. and J.B. Hillenbrand, "Heat Shunts and the Design of Energy-Efficient Evaporator Systems," Comp. & Chem. Eng., to appear (1987)

Wong, M.P.F. and J.D. Perkins, "Assessing Controllability of Chemical Plants", PSE '85: Process Systems Engineering, I. Chem. E. Symp. Ser. No. 92, p. 481, (1985)

No. Item	Optimum	Starting point	Lower bound	tapper bound
A., Objective Function ($\$10^6$/yr)	24.9286	20.659		
B., Design Variables				
1. Inlet temp, of reactor (°F)	400	400	400	600
2. Inlet temp, of 1st flash (°F)	65	65	65	100
3. Inlet temp, of 2nd flash (°F)	35	35	35	60
4. Inlet temp, of recyc. comp. (°F)	80.52	107	60	400
5. Purge fraction (%)	0.0085	0.01	0.005	0.1
6. Inlet pressure of reactor (psia)	2163.5	2000	1500	4000
7. Flowrate of feed 1 (lb xnol/hr)	2629.7	2632.0	2461.4	3000
8. Flowrate of feed 2 (lb xnol/hr)	691.78	691.4	643	1000
C,, Tear Variables				
1. Flowrate (lb mol/h)				
N_2	1494.8	1648		
H_2	3618.4	3676		
NH_3	524.2	424.9		
Ar	175.3	143.7		
CH_4	1989.1	1657		
2. Temperature (°F)	80.52	60		
3. Pressure (psia)	2080.4	1930		

Table 1. Result of ammonia optimization problem

Fig. 1. Ammonia Process Optimization



Max [before tax profit @ 15% over 5 years]

s.t. 100,000 tons NH_3/yr

No liquid In compressors

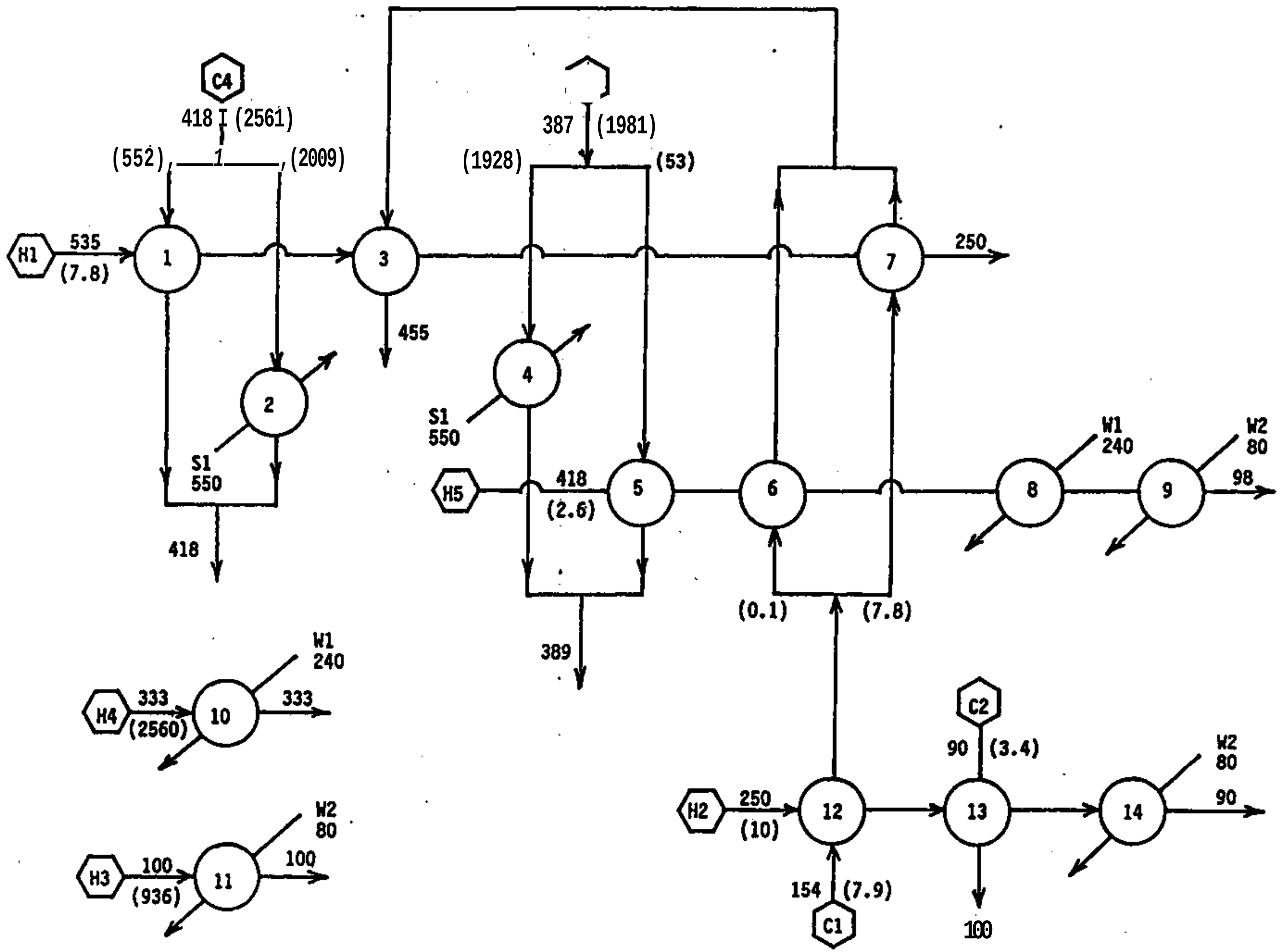
Product purity of % i 99.9X

Reactor temperature i 1000°F

NH_3 in purge $.4.5 lbn»1s/hr

1.8 * H_2/N_2 i 3.5

Fig. 2. Heat Exchanger Network for Ammonia Process



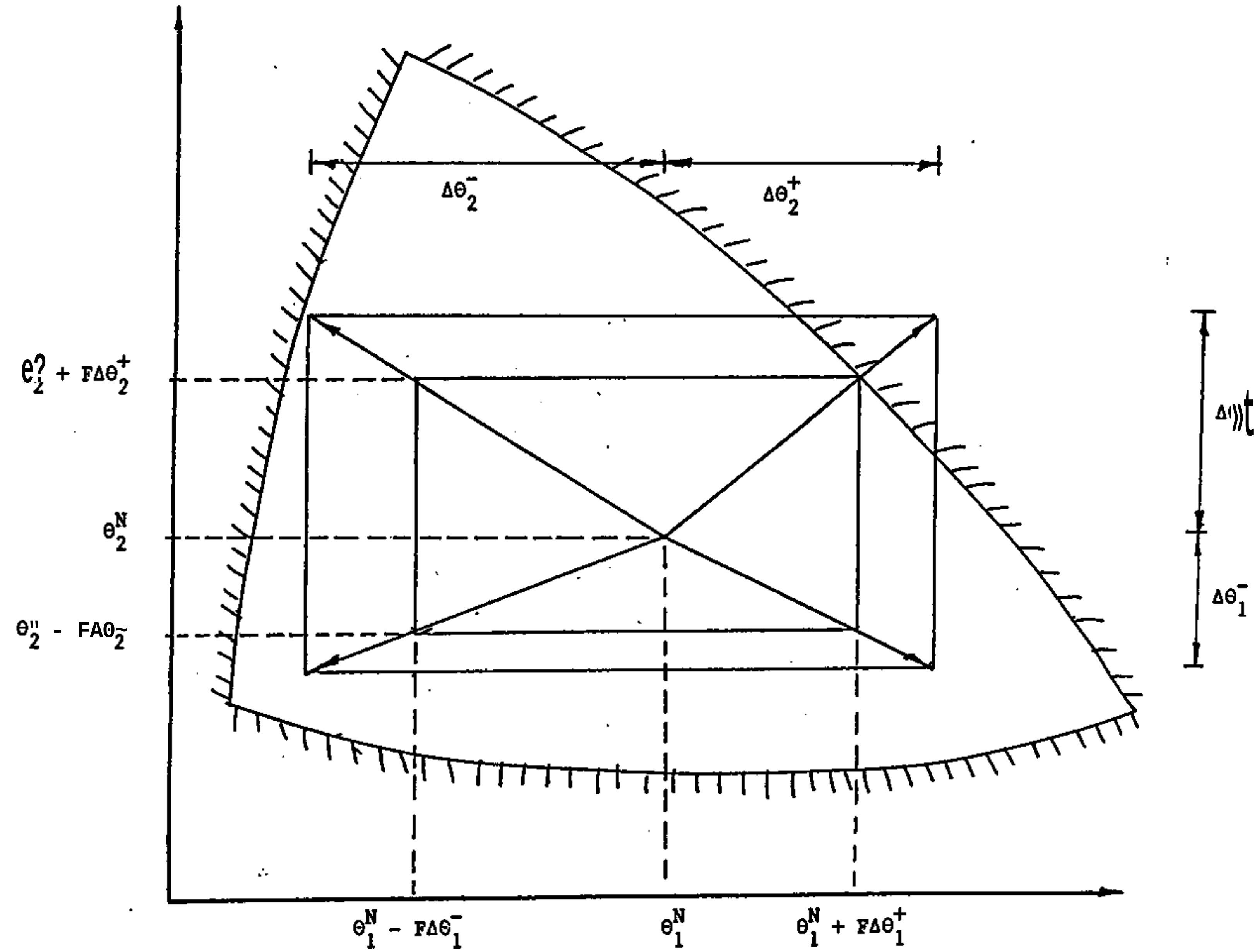


Figure 3. Evaluation of Flexibility

θ^N - nominal point for design
θ - uncertain parameters
F - flexibility index