FLEXPACK- A COMPUTER PACKAGE FOR OPTIMAL MULTIPERIOD DESIGN

by

A.I. Avidan & I.E. Grossmann

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A.I. Avidan and I.E. Grossmann

Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, Pa. 15213 U.S.A.

One of the main goals in chemical process design is to produce plant designs that are optimal with respect to a given economic performance index. Efforts to reach that goal have led to the development of computer-aided design techniques which allow the optimization of process flowsheets (Berna et al., 1980; Biegler and Hughes, 1982). While these techniques are often useful in practice, they have the important drawback that they may not produce flexible designs since they optimize the flowsheet for only a single nominal operating condition. That is, these techniques do not take explicitly into account the fact that once a design is implemented the plant will normally experience substantial variations in the operation. For example, in practice it is very likely that the plant will have to operate at various levels of capacity or to process different types of feedstocks. Therefore, by optimizing a flowsheet at a single nominal condition there is no guarantee that the plant will perform economically for other conditions, or even worse, that the plant will still be feasible to operate or able to meet desired specifications.

It is the purpose of this paper to describe a computer package for handling an important class of problems for the optimal design of flexible chemical plants. The problem that is addressed here is the one where a chemical plant must be designed optimally so as to operate in a specificed sequence of N time periods, where in each time period design parameters and specifications of the flowsheet may change. A general discussion on this design problem and its extensions to the problem of design under uncertainty can be found in Grossmann et al. (1982).

Multiperiod Design Problem

It will be assumed that a sequence of N time periods of fixed length t_i, $i=1,N$, is specified for the operation of a chemical plant. At each time period the plant operates at a different steady-state and dynamic effects of switching from one state to the other are neglected. The optimal design problem is then given by the following multiperiod nonlinear program

$$\min_{d, z^1, \ldots z^N} \quad C = C^0(d) + \sum_{i=1}^{N} C^i(d, z^i, x^i, t^i)$$

$$\text{s.t.} \quad \left.\begin{aligned} h^i(d, z^i, x^i, t^i) &= 0 \\ g^i(d, z^i, x^i, t^i) &\leq 0 \end{aligned}\right\} \quad i=1,N \qquad (1)$$

$$r(d) \leq 0$$

where

- C is the cost function that involves the investment cost C^0 and operating cost C^i for each period i
- d is the vector of design variables representing equipment sizes
- z^i is the vector of control variables in period i
- x^i is the vector of state variables in period i
- h^i, g^i are equality and inequality constraints that apply in each period i
- r is the vector of inequalities that involve the design variables

It should be noted that the vector of design variables d remains fixed throughout the periods of operation, whereas the control variables z^i represent the degrees of freedom in the plant operation. Since both types of variables, d and z^i, $i=1,N$, are decision variables to be optimized in problem (1), the difficulty that arises is that the computational burden in this problem can become excessive as the number of time periods increases.

Recently, Grossmann and Halemane (1982) have proposed a very efficient decomposition scheme that exploits two basic properties of problem (1). The first one is the block-diagonal structure in the constraints, which for fixed design variables d, allows the control variables z^i to be optimized independently for each time period. The second property is the fact that one can expect a large number of inequalities to be active or tight at the optimal solution. The proposed decomposition technique relies on a projection-restriction strategy in which the basic steps are as follows:

Step 1. Find a design d that is feasible to operate for the N time periods.

Step 2. (Projection). For the fixed design d, optimize the control variables z^i in each time period i, so as to improve the cost function and to identify inequalities $g_A^i=0$ that become active.

Step 3. (Restriction)

a) Eliminate control variables z_A^i from the active inequalities $g_A^i=0$ which are treated as equalities

b) Solve problem (1) in the restricted form

$$\min_{d, z_R^1, \ldots z_R^N} \; C = C^0(d) + \sum_{i=1}^{N} C^i(d, z_R^i, x_R^i, t^i)$$

$$\text{s.t.} \quad \left. \begin{aligned} h_R^i(d, z_R^i, x_R^i, t^i) &= 0 \\ g_R^i(d, z_R^i, x_R^i, t^i) &\le 0 \end{aligned} \right\} \quad i=1,N \qquad (2)$$

$$r(d) \le 0$$

where $z^i = (z_A^i, z_R^i)$, $x_R^i = (x^i, z_A^i)$, $h_R^i = (h^i, g_A^i)$, $g^i = (g_A^i, g_R^i)$.

Step 4. Return to Step 2 and iterate until there is no change in the design variables d.

As can be seen, the basic idea in this strategy is to conjecture in the projection step which inequalities are active at the solution, so that in the restriction step the original problem can be solved with a smaller number of control variables which are eliminated with the active inequalities. A detailed description of the projection-restriction strategy is given in Grossmann and Halemane (1982).

FLEXPACK

The projection-restriction strategy has been implemented in the computer package FLEXPACK (Avidan, 1982) which uses an equation oriented approach. The user specifies the multiperiod design problem as a nonlinear program with its corresponding objective function and constraint set. The constraints need not be written for each time period since in FLEXPACK they can be expressed in terms of parameters which take different values in each time period. Also, no gradient information has to be supplied since FLEXPACK uses numerical perturbations.

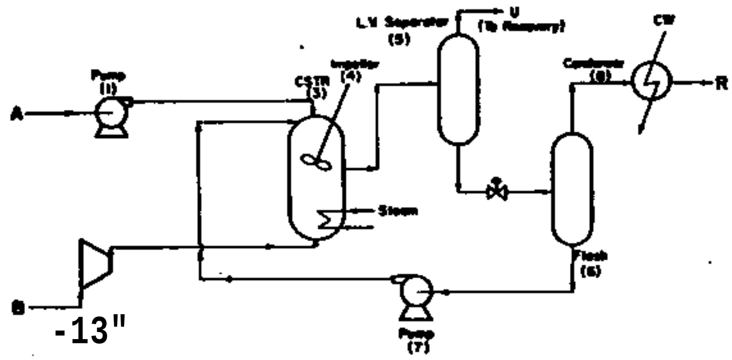
The system of equations in problem (1) is solved by using a tearing procedure which is also used to select the control variables z^i. This tearing procedure is a modification to Christensen's (1970) method in which a weighting scheme is used to specify preferred decision variables. In addition, this procedure incorporates the analysis of the reduced Jacobian matrix to ensure nonsingularity in the system of equations (see Halemane and Grossmann, 1981) which often becomes a critical issue when adding active inequalities to the restricted problem. For the numerical solution the single variable equations are solved with the inverse interpolation method by Shacham and Kehat (1972), whereas the torn variables are converged with Broyden's (1965) Quasi-Newton method. The variable-metric projection method of Sargent and Murtagh (1973) is used for solving the different optimization subproblems in the projection-restriction strategy. Specifically, this method is used for finding the initial feasible design in Step 1, for solving the optimization subproblems in the projection Step 2, and for solving the restricted problem in Step 3.

An important feature in FLEXPACK is that the user has the option to partition the design variables d into two sets: (a) the fixed variables d_f, (b) the capacity variables d_c. An example of the former are areas of heat exchangers, and an example of the latter are reactor volumes. Since the capacity variables are involved in inequalities of the form $d_c \geq d_c^i$, i=1,N, they are equivalent to $d_c = \max \{d_c^i,\ i=1,N\}$. Although it is well known that this max constraint is nondifferentiable, numerical experience with multiperiod problems that involve fixed time lengths t^i, has shown that the time period which defines the bottleneck for each capacity variable remains often unchanged throughout the iterations. Therefore, there are usually no numerical difficulties in using explicitly the max constraint which can be used to eliminate the capacity variables in the restricted problem so as to reduce further the size of this problem.

Numerical Example

The flowsheet shown in Fig. 1 has been optimized by considering N=1,2,...5, time periods of operation. In each period eight parameters such as temperatures of feedstream and of cooling water, product purity specifications, and efficiences are assigned different values. The details of the model and parameter values for this problem are given in Avidan (1982). This problem involves 8 design variables (7 of capacity type), 3N control variables, 31N equalities and state variables, and 6N inequalities. In all cases infeasible starting values were used. It is interesting to note that in the five cases studied there were always three inequalities that became active in the projection step so that all the control variables could be eliminated for the restriction step. In addition, by using max constraints for the seven capacity variables only one design variable

Fig. 1. Flowsheet of **example** problem



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(area of exchanger) had to be optimized in the restriction step.

The computer time requirements for the five problems solved are shown in Fig. 2. As can be seen the encouraging feature is that the total CPU-time increases only linearly in the number of periods, which is in agreement with the prediction of the computational model developed by Grossmann and Halemane (1982). Note that actually the projection step requires the largest time whereas the overhead for the equation ordering algorithm requires the smallest time. Also, as shown in Table 1, most of the computer time was spent in solving the systems of equations involved in the various steps of the decomposition strategy. These equations involve 4 or 5 tear variables.

Table 1. Computational Results

No. Periods	1	2	3	4	5
Total time* (sec)	46.2	102.1	148.4	193.9	233.9
Time for eqtn. solving* (sec)	42.1	94.9	138.6	181.1	218.3
No. eqtn. solutions	152	334	488	634	771

Conclusions

The projection-restriction strategy for optimal multiperiod design has been successfully implemented in the computer package FLEXPACK. As shown in the numerical example, the important feature is that the computer-time requirements only increase linearly in the number of periods. Thus, it is clear that this computer package provides the possibility of designing optimal flexible chemical proCesses with modest computational effort.

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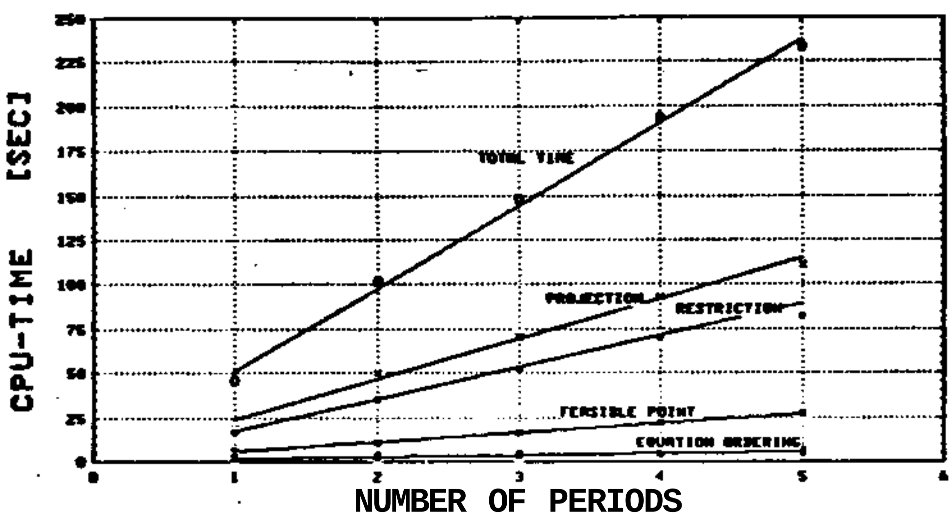

Fig. 2. CPU-time for different number of periods