A Direct Approach to Optimization of a Complex System

REIN LUUS and T. H. I. JAAKOLA

Department of Chemical Engineering and Applied Chemistry
University of Toronto, Toronto, Canada

Recently Adelman and Stevens (1972) applied a constrained simplex method to optimize the design of a chemical plant which consisted of a continuous stirred tank reactor, a heat exchanger, a decanter, and a distillation column. The operation of the plant is described by 9 equations in 13 variables—F_A, F_B, F_D, F_G, F_P, F_{RA}, F_{RB}, F_{RC}, F_{RE}, F_{RP}, F_R, V, and T. The authors fixed one variable F_P at the value 4763 and then considered the optimization of the plant as a nonlinear programming problem. The objective function to be maximized is percent return from the plant.

The purpose of this communication is to point out that the mass balance equations are not all independent and that the equations can be rearranged to provide a simple means of solution. Also, we wish to show that the optimal performance index does not change if F_P is allowed to change, provided that the other variables are allowed to take on new optimal values. In order that the reader may make a direct comparison, we use the same notation as was used by Adelman and Stevens.

The 9 equations of Adelman and Stevens may be put into a convenient form if we group the terms by introducing 3 groups of variables. These are chosen to be

$$\beta = V\rho/F_R^2 \tag{1}$$

$$b = F_{RP} - 0.2(4\beta k_2 F_{RB} F_{RC} - 2.5\, k_3 \beta F_{RC} F_{RP}) \tag{2}$$

and

$$\alpha = F_{RA} + F_{RB} + F_{RC} + 11b \tag{3}$$

With these definitions, the 9 constraint equations become

$$F_G = 1.5 k_3 F_{RC} F_{RP} \beta \tag{4}$$

$$F_{RA} = \frac{F_{RC}}{10 k_1 F_{RB}} (10 k_2 F_{RB} + 5 k_3 F_{RP} + k_2 F_{RB} F_{RC}/b) \tag{5}$$

$$F_P = F_{RP} - b \tag{6}$$

$$F_D = 0.2 \alpha \beta k_2 F_{RB} F_{RC}/b \tag{7}$$

$$F_A = k_1 F_{RA} F_{RB} \beta + F_D F_{RA}/\alpha \tag{8}$$

$$F_B = F_G + F_P + F_D - F_A \tag{9}$$

$$F_R = \alpha + F_G + F_P \tag{10}$$

$$F_{RE} = 10(F_{RP} - F_P) \tag{11}$$

The reader can readily verify that these 8 equations, namely Equations (4) to (11), are equivalent to Equations (15) to (23) of Adelman and Stevens.

For the purposes of optimization, let us take as the independent variables T, F_{RC}, F_{RP}, β, and F_{RB}. If values are given to these variables, then all the other variables can be calculated seriatim. The calculations may be followed in the following series:

1. Evaluate k_1, k_2, k_3.
2. Evaluate F_G from Equation (4).
3. Evaluate b from Equation (2).
4. Evaluate F_{RA} from Equation (5).

TABLE 1. SOLUTIONS TO PLANT OPTIMIZATION

Variable	Present optimal solution	Solution of Adelman and Stevens	Corrected solution of Adelman and Stevens
F_A	13,516.20	13,338.52	13,508.20
F_B	30,782.36	30,759.72	30,656.17
F_D	36,321.90	36,159.42	36,224.43
F_{RA}	47,645.34	45,977.96	46,556.53
F_{RB}	147,433.81	142,784.52	142,784.52
F_{RC}	7,808.55	7,725.44	7,725.44
F_{RE}	145,962.99	141,919.98	141,914.02
V	30.71	32.01	32.11
F_R	371,423.65	360,538.72	361,111.84
F_{RP}	19,360.26	18,955.00	18,955.00
T	674.44	672.61	672.61
F_G	3,212.70	3,175.82	3,176.35
F_P	4,763.96	4,763.00	4,763.60
P	121.53	121.66	121.33

TABLE 2. EFFECT OF β ON SOLUTION TO THE OPTIMIZATION PROBLEM

Variable	$\beta = 1.16 \times 10^{-10}$	$\beta = 2.51 \times 10^{-9}$	$\beta = 1.12 \times 10^{-8}$	$\beta = 4.58 \times 10^{-8}$	$\beta = 3.58 \times 10^{-6}$
F_A	1,295,050.48	59,636.95	13,502.90	3,337.01	42.65
F_B	2,953,069.66	136,007.92	30,769.34	7,601.89	97.16
F_D	3,483,024.91	160,409.39	36,299.64	8,968.86	114.63
F_{RA}	4,557,623.83	209,935.42	47,422.71	11,689.54	149.50
F_{RB}	14,148,319.20	651,929.50	146,960.25	36,202.00	462.91
F_{RC}	746,495.58	34,381.60	7,773.54	1,917.72	24.52
F_{RE}	13,997,709.48	644,907.92	145,452.98	35,847.84	458.39
V	2,941.59	135.41	30.74	7.62	0.09736
F_R	35,615,014.27	1,640,880.71	370,127.38	91,211.92	1,166.34
F_{RP}	1,856,611.88	85,530.14	19,306.46	4,761.41	60.88
T	674.54	674.56	674.41	674.28	674.30
F_G	308,254.30	14,196.13	3,211.44	793.41	10.14
F_P	456,840.93	21,039.35	4,761.16	1,176.62	15.04
P	121.53	121.53	121.53	121.53	121.53

5. Evaluate α from Equation (3).
6. Evaluate F_P, F_D, F_A, F_B, F_R, and F_{RE} seriatim from Equations (6) to (11).
7. Evaluate V from Equation (1).

As can be seen, the calculational procedure for obtaining values for all variables is straightforward and no iterative procedure is necessary. Also, no extraneous solutions result.

The objective function to be maximized is the percent return given by

$$P = (84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R - 60V\rho)/(6V\rho) \quad (12)$$

In order to compare the results directly to the solution obtained by Adelman and Stevens (1972), we introduce an inequality constraint

$$4762 \leq F_P \leq 4764 \quad (13)$$

To carry out the maximization, we used a direct search procedure employing pseudo random numbers and search region contraction. We will outline this procedure and apply it to more complicated optimization problems in another paper. The computations were performed in double precision and the optimum was obtained in 5 sec. of computation time on an IBM 370/165 digital computer. In Table 1 we present the results and also the solution obtained by Adelman and Stevens. In the last column of the table we have corrected their solution by assuming F_{RB}, F_{RC}, F_{RP}, T, and β to be correct and then adjusting the other variables in the solution so that all the constraint equations are satisfied. Thus the optimal value of 121.53 obtained by us should be compared to 121.33 and not 121.66.

Now let us relax the inequality constraint given by Equation (13) and look at the effect of allowing F_P to be a free variable. We performed the optimization procedure with several widely different starting conditions, but always the same maximum value of $P = 121.534$ was obtained. However, the optimum is not uniquely defined, and in the optimization one flow-rate variable or volume can be fixed and a search may be performed on the remaining 4 variables.

Therefore we chose some values for β and carried out optimization with respect to the remaining variables T, F_{RC}, F_{RP}, and F_{RB}. Table 2 contains 5 sets of results from $\beta = 1.16 \times 10^{-10}$ to $\beta = 3.58 \times 10^{-6}$. It should be noted that the maximum value of P is the same at 121.53 even when F_P changes over a very wide range.

Once again we emphasize that the optimal solution was so readily obtained mainly because of the realization that there are 5 independent variables in the problem. This allowed all the variables to be calculated seriatim and exactly and it was not necessary to use a numerical procedure to solve approximately any algebraic equation.

ACKNOWLEDGMENT

This work was performed with the assistance of a grant from the Canadian National Research Council, A-3515. Computations were carried out with the facilities of the University of Toronto Computer Center.

LITERATURE CITED

Adelman, A., and W. F. Stevens, "Process Optimization by the Complex Method," *AIChE J.*, 18, 20 (1972).

Manuscript received December 12, 1972; revision received January 15 and accepted January 16, 1973.

Perfect-Mixing Approximation of Imperfectly Mixed Continuous Crystallizers

EUGENE B. LIEB

Department of Chemical Engineering
University of Rochester, Rochester, New York 14627

Theoretical models for the continuous tank crystallizer have rested heavily on the assumption of perfect mixing (Randolph, 1971). However, no assumption is more intractable either theoretically or experimentally. Accordingly, the fact that modeling of continuous crystallizers has seemed to be successful in describing some behavior is surprising. The general model of the perfectly mixed tank crystallizer developed by Randolph and Larson (1971), Stone and Randolph (1969), Hulbert and Stefango (1969), and Sherwin et al. (1969) centers around a balance on the population of crystals. With appropriate auxiliary conditions this balance yields the crystal size distribution in terms of the growth rate of a characteristic linear dimension of the crystals. The perfect mixing assumption enters into the development of the population balance by the specification that only one unique