Evaluating Significant Economic Trade-Offs for Process Design and Steady-State Control Optimization Problems

An order-of-magnitude analysis that evaluates the significant economic trade-offs for the process design optimization problem allows rapid screening of flowsheet alternatives. The optimization problem is simplified by eliminating all but the most important design variables and by including only the dominant cost functions for each trade-off. Quantitative parameters are defined which allow a straightforward selection of these elements and identify the incentive for optimization. A new optimization criterion helps to prevent the rigor of the optimization analysis from exceeding the accuracy of the design and economic models used.

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SCOPE

There are numerous flowsheets that can be generated for any chemical process (Douglas, 1985), and there are ten to twenty optimization variables for each flowsheet (Westerberg, 1981). This paper describes a shortcut optimization procedure that is useful for screening flowsheet alternatives, as well as for subsequent design optimizations. The procedure addresses the following topics: (1) Identifying the most important design variables for optimization; (2) using only the cost functions that dominate the economic trade-offs for these variables; (3) identifying the incentive for optimization; and (4) preventing the rigor of the optimization from exceeding the accuracy of the design and economic model. Each of these criteria is defined quantitatively in the proposed formulation.

CONCLUSIONS AND SIGNIFICANCE

The optimization of a process design variable is characterized by a trade-off between monotonically increasing and monotonically decreasing cost functions, so that the optimization problem is usually unimodal and is seldom constrained. An order-of-magnitude reduction in the computational requirements to estimate the optimum can be obtained simply by eliminating all of the cost factors in the total annualized cost function whose gradients are an order of magnitude less than the largest (positive and negative) values. A rank-order parameter is defined which quantitatively identifies the most significant optimization variables (so that the unimportant design variables can be eliminated from the analysis). Also, a proximity parameter is defined that indicates how far a base-case value of a design variable is from its optimum value (before the optimum has been determined). These simplifications of the optimization analysis are particularly useful for screening calculations where a choice is being made among a large number of process alternatives.

INTRODUCTION

There is a vast literature concerned with optimization theory. In recent reviews, Sargent (1980) points out that the literature is growing at an enormous rate, and Westerberg (1981) states, "a thorough review is impossible." However, virtually all of this literature is focused on the mathematics of optimization (i.e., developing very general, robust procedures). There has been little effort devoted to the development of very efficient optimization routines that are specific to process optimization problems. The purpose of this paper is to describe an alternative approach for finding nearly optimum designs for chemical processes.

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PROCESS OPTIMIZATION FOR SCREENING CALCULATIONS

In the initial stages of a process design it is possible to generate on the order of one million flowsheets (Douglas, 1984). Each flowsheet is described by tens of thousands of equations and a like number of inequality constraints, and there are normally ten to twenty optimization variables (Westerberg, 1981). It does not appear likely that the "structural parameter" approach to determine the optimum flowsheet structure and the optimum design conditions simultaneously will be able to handle problems of this magnitude in the foreseeable future. (See Westerberg, 1981, and Nishida et al., 1981, for more complete discussions of this approach.) Thus, some preliminary screening is necessary.

In this paper we outline an alternative optimization procedure that provides an efficient way of screening the process alternatives that can be generated using the hierarchical decision procedure described by Douglas (1985). It should be emphasized that the calculations and the optimizations associated with screening do not have to be rigorous. All that we require is sufficient accuracy so that we can discard the poor flowsheet alternatives. Therefore the initial analysis is based on: (1) approximate material and energy balances, (2) simple design and economic models, and (3) an order-of-magnitude optimization analysis.

ECONOMIC TRADE-OFFS: IDENTIFYING AND CHARACTERIZING DESIGN VARIABLES

Process design optimization problems can be characterized by an economic trade-off between monotonically increasing cost functions and monotonically decreasing cost functions. For example, the well-known problem of determining the optimum reflux ratio for a distillation column balances a rapidly increasing column cost as the minimum reflux ratio is approached vs. slowly increasing costs for steam, cooling water, the reboiler, and the condenser as reflux ratio is increased (Peters and Timmerhaus, 1980). Similar economic trade-offs for other design problems can be identified, and the resulting optimizations are virtually always unimodal. Moreover, while these variables may have physical limits (e.g., $R > R_{min}$), their optimum values are almost never constrained.

Process Flow vs. Unit Optimizations

We define a process flow optimization to be the optimization of a variable that has a significant impact on the input and output flowrates (i.e., the product distribution) or the recycle flowrates for the process. Generally, these variables will also affect the capital and operating costs of each piece of equipment either in a direct path through the process or in a recycle loop. Unit optimizations, on the other hand, affect the design of only a single piece or a few adjacent pieces of equipment. Common design variables corresponding to these categories are as follows.

Common Design Variables in Petrochemical Processes

Process Flow Optimization Variables

1. Reactor conversion
2. Reactor temperature
3. Reactor pressure
4. Molar ratio of reactants at reactor inlet
5. Purge composition

Unit Optimization Variables

1. Reflux ratio in distillation columns
2. Solvent flowrate in gas absorbers
3. Fractional recovery in distillation columns or gas absorbers
4. Approach temperature in heat exchanger networks
5. Flash drum temperature
6. Flash drum pressure
7. Distillation column pressure

The process flow optimization variables determine the selectivity (moles of desired component produced per mole of reactant converted) or product distribution for the process, in addition to having a major impact on the internal process flows and equipment costs. Thus we expect most of these variables to be significant design variables. It is interesting to note, however, that there are no reliable rules of thumb available for selecting values for any of these variables. For example, reactors are often designed to maximize yield (moles of product at the reactor outlet per mole of reactant at the reactor inlet). However, these conditions will never correspond to the reactor design which maximizes the profitability of the process. Thus, in order to compare flowsheet alternatives some optimization procedure is required to estimate the optimum flows and equipment sizes.

It should not be surprising that no heuristics have been proposed for specifying values of the process flow optimization variables. These variables have a significant impact on most of the equipment and operating costs, but the dominant trade-offs for each variable are dependent upon the process under consideration. The optimum design of reactors is particularly difficult to generalize because of the wide range of complex chemistry encountered in petrochemical process. For example, as the reactor temperature is increased above ambient conditions, the heating and cooling costs will increase while the reactor cost will decrease. The selectivity losses may either increase or decrease, however, depending upon the complex reaction kinetics.

There are also a large number of unit optimization variables for any process, as noted in the list of design variables above. In most cases these variables can be specified using well-known rules of thumb. Moreover, the economic trade-offs involved with these variables are more easily generalized, rather than being flowsheet specific. The common trade-offs for these variables are given below. It is not clear whether a particular unit optimization variable is "significant," however, or whether a heuristic provides a reasonable estimate of its optimum value. The quantitative procedure described below has been developed to specify which of these variables should be optimized for flowsheet screening calculations.

Economic Trade-Offs and Heuristics for Unit Optimization Variables in Petrochemical Processes

Reflux ratios in distillation columns. Trades off number of trays required for a given separation vs. steam and cooling water costs, reboiler and condenser area, and column diameter.

Heuristic: $R = 1.2R_{min}$

Solvent flowrate in gas absorbers. Trades off number of trays required for a given recovery of solute vs. solvent recovery costs.

Heuristic: $L/mG = 1.4$ for isothermal, dilute systems

Fractional recovery in distillation columns or gas absorbers. Trades off number of column trays vs. economic penalty for poor recovery of solute or key component (losses to waste stream, incremental recycle costs, increased difficulty of downstream separations, etc.)

Heuristic: >99% recovery of valuable components

Approach temperature in a heat exchanger network. Trades off heat exchanger area vs. process heating and cooling (utilities) costs.

Heuristic: Develop the heat exchanger network using a ten degree approach temperature at the pinch for temperatues in the range from ambient to 533 K (500°F).

Flash drum temperature. Trades off the flash drum cooler area vs. the load on the vapor recovery system (or the losses of valuable components in a purge stream if no recovery system is used).

$$\text{Heuristic: } T_{\text{flash}} = T_{\text{cw}} + 5\text{ K}$$

Flash drum pressure. Trades off increased equipment costs for high pressure operation vs. vapor recovery system duty or purge losses.

Heuristic: Maintain $K_1 < 0.1$ for all heavy components.

Distillation column pressure (for partial condensers). Trades off increased equipment costs for high pressure operation vs. losses of valuable components in the partial condenser vent stream.

Heuristic: Recovery 99% of the valuable components in the liquid distillate stream.

COST MODEL FOR A COMPLETE PLANT

In order to characterize the design optimization problem, we must develop a cost model for the process in terms of the design variables of interest. For screening calculations we use approximate material balances, equipment design procedures, and cost correlations to develop the process cost model. The shortcut equipment design procedures used are similar to those described by Glinos and Malone (1984) for estimating the minimum reflux ratios in distillation columns.

The cost models are developed with respect to a base-case design for each flowsheet alternative. We assume that all equipment designs are continuous functions (i.e., heat exchangers are available with any area, distillation columns are available for any height and diameter, etc.). The cost correlations we use are those published by Guthrie (1969). Since the process cost models we develop are quite simple, we can easily determine the sensitivity of the total processing costs to changes in the design parameters, such as overall heat transfer coefficients, reaction kinetic parameters, tray efficiencies, and similar factors.

Equipment Cost Models. Once the material and energy balances have been estimated, we can calculate the equipment costs from the base-case process flows and equipment costs. For example, the installed cost of a heat exchanger can be written as

$$\frac{C}{C_{BC}} = \left(\frac{A}{A_{BC}}\right)^{0.65} \tag{1}$$

where we are using the cost exponent from Guthrie (1969). The exchanger area can then be calculated from

$$Q = FC_P\Delta t \tag{2}$$

The ratio of areas can be related to the base-case conditions as follows

$$\frac{A}{A_{BC}} = \frac{F\Delta t}{(F\Delta t)_{BC}}\frac{\Delta T_{m,BC}}{\Delta T_m} \tag{3}$$

Substituting this result into Eq. 1 gives the desired relationship between the heat exchanger cost and the process flows and temperatures. Similar cost fuctions for other equipment types are easily developed (see Appendix A).

It is now apparent that a reasonable base-case design is required. The equipment cost correlations are only valid for equipment sizes reasonably close to the base-case sizes. Nonetheless, cost correlations such as those found in Guthrie (1969) are valid over a large enough range for our preliminary optimizations. In the unusual case that models are not applicable (e.g., $A/A_{BC} > 10$), a new base-case design should be developed.

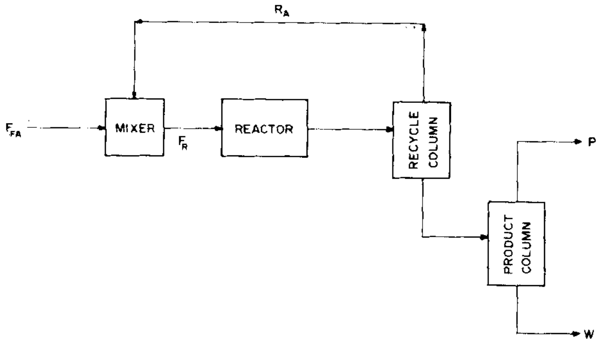

Figure 1. Flowsheet for the reaction system $A \rightarrow P \rightarrow W$.

Utilities Costs. The utilities costs are also easily related to the base-case costs once the process flows have been estimated. For example, the heat balance for a water cooler is given by

$$FC_P\Delta t = F_{\text{cw}}C_{P,\text{cw}}\Delta t_{\text{cw}} \tag{4}$$

The cooling water cost can then be related to the base-case value by

$$\frac{C_{\text{cw}}}{C_{\text{cw},BC}} = \frac{F_{\text{cw}}}{F_{\text{cw},BC}} = \frac{F\Delta t}{(F\Delta t)_{BC}} \tag{5}$$

Process Economic Model. Now we can write an expression for the profit of a process

$$\begin{aligned}\text{Annual Profit} &= (\text{Product value}) + (\text{By-product value}) \\ &\quad - (\text{Raw material costs}) - (\text{Annualized capital costs} \\ &\quad \text{for all units}) - (\text{Operating costs for all units})\end{aligned} \tag{6}$$

The installed equipment costs are put on an annualized basis by multiplying them by a capital charge factor (say, one-third year for petrochemical processes). When we are comparing process alternatives we include only the significant items on the flowsheet in this calculation; i.e., we neglect the cost of pumps, flash drums, reflux drums, etc. By substituting the expressions for equipment and utilities costs for the various process costs into Eq. 6, we can develop a simple economic model in terms of our significant design variables.

EXAMPLE

A flowsheet for the simple reaction system

$$A \rightarrow P \rightarrow W \tag{7}$$

is shown in Figure 1. Component P represents the desired product and W is a waste by-product. The kinetics of both reactions are first-order with activation energies $E_1 < E_2$. The relative volatilities are such that $\alpha_A > \alpha_P > \alpha_W$, and we assume that the direct column sequence is favorable. The product stream flowrate and composition are specified, but the composition of the waste stream corresponds to a design optimization variable. The other optimization variables we wish to consider are the reactor conversion and temperature and the reflux ratio for the product column. Several other design variables are available for this process (which ordinarily should be evaluated), but we have neglected them to simplify the presentation of this example.

Thirteen cost functions are included in the economic model for this process (see Appendix B for derivation of cost model). The profit expression is given by:

TABLE 1. SUMMARY OF COST FUNCTIONS FOR EXAMPLE REACTOR SYSTEM

i	f_i	Cost, \$ million/yr
1	Fresh feed	$\frac{25{,}012}{f_P S} - 25{,}012$
2	Waste (credit)	$-1{,}630 \frac{(0.999 - f_P S)}{f_P S}$
3	Reactor	$16.68 \left[\frac{\ln(1/1 - x)}{k_1 x f_P S}\right]^{0.623}$
4	Col 1 shell	$45.6 \left[\frac{1 - 0.842x + 0.316xS}{f_P x S}\right]^{0.533}$
5	Col 1 cond	$15.8 \left[\frac{1.9 - 1.6x + 0.6xS}{f_P x S}\right]^{0.65}$
6	Col 1 cw	$5.15 \left[\frac{1.9 - 1.6x + 0.6xS}{f_P x S}\right]$
7	Col 1 reb	$12.47 \left[\frac{1.9 - 1.6x + 0.6xS}{f_P x S}\right]^{0.65}$
8	Col 1 stm	$87.1 \left[\frac{1.9 - 1.6x + 0.6xS}{f_P x S}\right]$
9	Col 2 shell	$5.63 \ln \left[\frac{x_{D,P}(1 - S) - (1 - x_{D,P}) f_P S}{(1 - x_{D,P})(1 - f_P) S}\right]^{0.802} \left[\frac{R/R_m + S}{S}\right]^{1.066}$
10	Col 2 cond	$15.6 \left[\frac{R/R_m + S}{S}\right]^{0.65}$
11	Col 2 cw	$5.63 \left[\frac{R/R_m + S}{S}\right]$
12	Col 2 reb	$16.23 \left[\frac{R/R_m + S}{S}\right]^{0.65}$
13	Col 2 stm	$88.0 \left[\frac{R/R_m + S}{S}\right]$

Where:
$k_1 = 5.35 \times 10^{10} \exp(-9{,}050/T_R)$
$k_2 = 4.61 \times 10^{17} \exp(-15{,}100/T_R)$
$S = \left(\frac{1}{x}\right)\left(\frac{1}{1 - k_1/k_2}\right)[(1 - x)^{k_1/k_2} - (1 - x)]$
$x_{D,P} = 0.999$

Profit = (Product value) + (Waste by-product credit)
− (Raw materials) − (Reactor) − (Column 1 shell)
− (Column 1 condenser) − (Column 1 coolant)
− (Column 1 reboiler) − (Column 1 steam)
− (Column 2 shell) − (Column 2 condenser)
− (Column 2 coolant) − (Column 2 reboiler)
− (Column 2 steam) (8)

By subtracting the difference between the product value and the minimum raw material costs (i.e., the cost of the minimum amount of A required by the stoichiometry of Eq. 7), we obtain an expression for the total annual processing costs (TAC). This expression has the form

$$\text{TAC} = f_1 + f_2 + \ldots + f_n \quad (9)$$

The cost functions for this example are given in Table 1.

PRELIMINARY OPTIMIZATION ANALYSIS

If there are n terms in the cost expression above and m design variables, we can write the conventional optimization equations

$$\delta\text{TAC} = \frac{\partial \text{TAC}}{\partial x_1}\delta x_1 + \ldots + \frac{\partial \text{TAC}}{\partial x_m}\delta x_m = 0 \quad (10)$$

or

$$\delta\text{TAC} = \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_1}\delta x_1 + \ldots + \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_m}\delta x_m = 0 \quad (11)$$

In order to screen our flowsheet alternatives, we would like a procedure for obtaining a "reasonable" estimate of the optimum values of each of the design variables. There will be heuristics for specifying values for most of the unit optimization variables, but we may still want to calculate their optimum values. There is no way of guessing the optimum process flows, however. Again, we can simplify our evaluation of Eq. 11 by eliminating unimportant cost functions (f_i's) and design variables (x_j's).

Scaling

We could evaluate the relative importance of the variables by comparing ($\partial\text{TAC}/\partial x_j$) for each variable at some base-case design conditions. Unfortunately, Eq. 10 is very poorly scaled, so this comparison would yield misleading conclusions. By estimating the

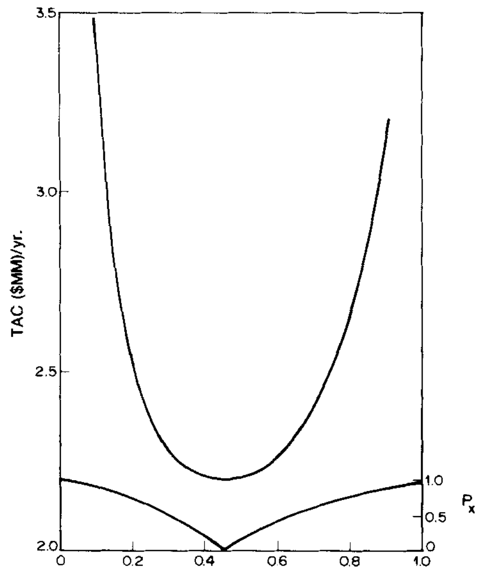

Figure 2. Effect of design value for conversion on total annualized cost and proximity parameter; all other design variables held at optimum values.

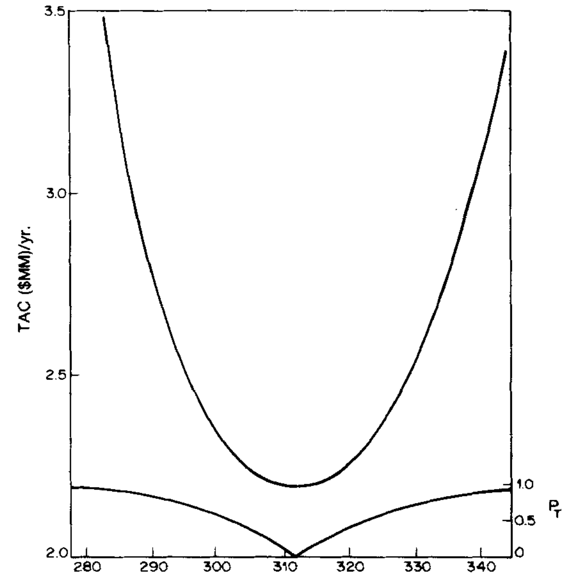

Figure 3. Effect of design value for reactor temperature on total annualized cost and proximity parameter.

range of values over which each variable should be considered, $\Delta x_{j,\max}$, we can write

$$\Delta \mathrm{TAC}_{\max} = \frac{\partial \mathrm{TAC}}{\partial x_1} \Delta x_{1,\max} + \ldots + \frac{\partial \mathrm{TAC}}{\partial x_m} \Delta x_{m,\max} \quad (12)$$

Now, by comparing $(\partial \mathrm{TAC}/\partial x_m \, \Delta x_{j,\max})$ for each design variable, we could eliminate those variables which have only a small potential for reducing the annualized costs.

It should be noted that the values selected for $\Delta x_{j,\max}$ generally have some physical significance. The range of reactor temperatures and pressures to be considered will be available from the chemist (or the patent literature), fractional recoveries in separation units are expected to be between 0.99 and 1.0, and reflux ratios might vary from $R/R_m = 1.01$ to 1.3. The range of conversions for complex reactions probably falls in the range from 0.1 to the conversion corresponding to the maximum yield, purge compositions of reactants are probably in the range from 0.1 to 0.9, etc.

Of course, the values for some of the primary design variables may be fortuitously close to their (local) optimum at base-case conditions. If an unimportant variable is far from its optimum, it will appear to be more important. Thus, selection of variables for optimization using Eq. 12 may still be inadequate.

Rank-Order and Proximity Parameters

Alternatively, we define the rank-order parameter for each design variable to be

$$r_j = \sum_{i=1}^{n} \left| \frac{\partial f_i}{\partial x_j} \right| \Delta x_{j,\max} \quad (13)$$

The important advantage of this parameter is that its value is quite insensitive to the base-case design conditions. That is, even if $(\partial \mathrm{TAC}/\partial x_j)$ is nearly zero at the base-case, r_j still indicates the relative importance of the design variable x_j. If the rank-order parameter for any design variable is an order of magnitude smaller than the largest value, this variable is eliminated from the optimization analysis for screening calculations.

We can also reduce the calculations required for screening flowsheet alternatives by preventing the rigor of the optimization procedure from exceeding the accuracy of the design and economic models used. We define the proximity parameter

$$p_j = \frac{\left| \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_j} \right|}{\sum_{i=1}^{n} \left| \frac{\partial f_i}{\partial x_j} \right|} \quad (14)$$

which quantifies the closeness of x_j to its optimum value, and thus is quite sensitive to the base-case conditions. The important property of p_j is that it approaches zero at $x_{j,\mathrm{opt}}$ and approaches unity as x_j moves away from the optimum. Hence, p_j provides an important measure of the proximity of x_j to $x_{j,\mathrm{opt}}$, even though $x_{j,\mathrm{opt}}$ is not known.

In Figures 2 to 5, the relationship between p_j and x_j is illustrated for each of the four design optimization variables in our previous example. These plots support an important heuristic for our flowsheet screening calculations.

Optimize the most important design variables only until $p_j < 0.5$ *for each* x_j.

This criterion is implemented because it insures reasonable optimality for our design without exceeding the accuracy of the design and economic models.

EXAMPLE (CONTINUED)

In Table 2 we show the calculated values of $\partial f_i/\partial x_j$, $\partial \mathrm{TAC}/\partial x_j$, r_j, and p_j at base-case design conditions for our example above ($x = 0.8$, $T_R = 305$ K, $f_P = 0.995$, and $R/R_m = 1.2$). The gradients appear to indicate that the economic importance of the variables is in the order

$$f_P > x > R/R_m > T_R$$

whereas the scaled gradients, $(\partial \mathrm{TAC}/\partial x_j \, \Delta x_{j,\max})$, indicate that the order is

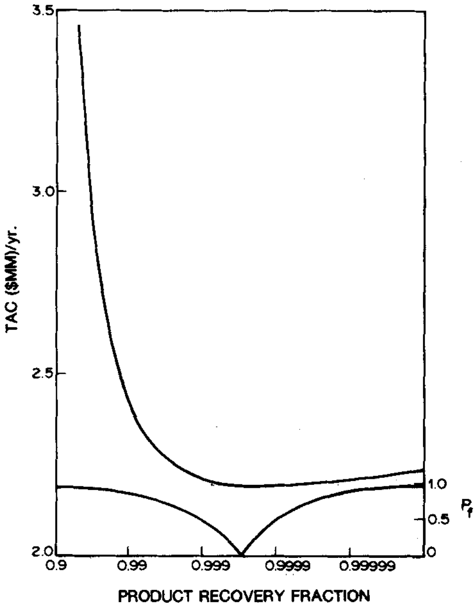

Figure 4. Effect of design value for recovery fraction (of component *P* overhead in product column) on total annualized cost and proximity parameter.

$$x > f_P > T_R > R/R_m$$

However, the rank-order parameter indicates that the proper order should be

$$x, T_R > f_P > R/R_m$$

By noting the rank-order parameter and proximity parameter for each variable, we can classify our base-case design as follows

x	Important variable	Far from optimum
T_R	Important variable	Close to optimum
f_P	Less important variable	Far from optimum
R/R_m	Unimportant variable	Roughly optimum

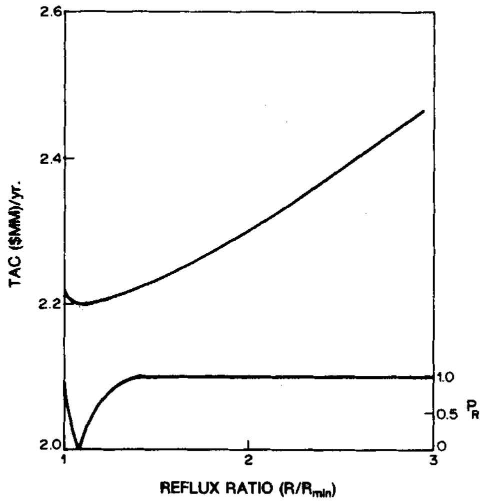

Figure 5. Effect of design value for reflux ratio on total annualized cost and proximity parameter.

Approximate Optimization

Table 2 clearly indicates the economic trade-offs associated with each design variable. That is, the terms with positive or negative gradients are associated with the monotonically increasing or decreasing cost functions. We can perform an order-of-magnitude analysis by neglecting all positive terms for each design variable that are an order of magnitude smaller than the largest positive term, and the same for the negative terms. The dominant trade-offs for the design variables in our example problem are then:

x	Raw material cost vs. Steam for recycle column
T_R	Raw material cost vs. Reactor cost
f_P	Raw material cost vs. Product column shell cost
R/R_m	Steam for column vs. Product column shell cost

Thus, we should be able to obtain a reasonable estimate of the optimum design by calculating only five cost functions instead of 13,

TABLE 2. GRADIENTS OF COST FUNCTIONS WITH RESPECT TO DESIGN VARIABLES: $ MILLION/YR

f_i	$\frac{\partial f_i}{\partial x}$	$\frac{\partial f_i}{\partial T_R}$	$\frac{\partial f_i}{\partial f_P}$	$\frac{\partial f_i}{\partial (R/R_m)}$
Feed	2,150.0	37.6	−25,800.0	0.0
Waste	−69.0	−1.3	825.0	0.0
Reactor	689.0	−34.0	−357.0	0.0
Column 1	−44.0	0.02	−21.0	0.0
Condenser 1	−25.0	0.002	−9.0	0.0
Coolant 1	−15.0	0.005	−7.0	0.0
Reboiler 1	−21.0	0.009	−10.0	0.0
Steam 1	−260.0	0.1	−122.0	0.0
Column 2	38.0	0.5	1,610.0	−29.6
Condenser 2	0.8	0.01	0.0	7.8
Coolant 2	0.6	0.01	0.0	5.7
Reboiler 2	0.8	0.008	0.0	8.2
Steam 2	9.0	0.2	0.0	90.0
$\partial TAC/\partial x_j$	2,450.0	3.2	−23,900.0	82.1
$\Delta x_{j,max}$	0.2	10.0	0.005	0.2
$(\partial TAC/\partial x_j)\Delta x_{j,max}$	490.0	32.0	120.0	16.4
r_j	660.0	740.0	140.0	28.3
p_j	0.74	0.04	0.86	0.58

TABLE 3. RESULTS OF APPROXIMATE AND RIGOROUS DESIGN OPTIMIZATIONS

	Case I	Case II	Case III	Case IV
x	0.80	0.448	0.40	0.40
T_R	305.0	311.8	312.7	312.6
f_p	0.995	0.9997	0.9997	0.9997
R/R_m	1.20	1.07	(1.20)	1.09
TAC ($ million)/yr	2,649.0	2,197.0	2,212.0	2,205.0
ΔTAC,%	20.5	0.0	0.7	0.4

Case I = base-case.
Case II = rigorous optimum.
Case III = approximate, three-variable optimum ($R = 1.2R_m$).
Case IV = approximate, four-variable optimum.

and only eight derivatives instead of 52 (assuming that we consider all four optimization variables).

The results of the approximate optimization analysis are given in Table 3, and are compared to the exact optimum. The optimum design is 17% cheaper than the base-case design, but only 0.4% less expensive than the approximate optimum design.

Because the rank-order parameter for the design reflux ratio was an order of magnitude smaller than the largest value, we could have eliminated this design variable from the screening optimization. Even though only four cost functions and six derivatives were evaluated, the resulting design was only 0.7% more expensive than the rigorous optimum given in Table 3.

RIGOROUS OPTIMIZATION ANALYSIS

After several candidate flowsheets have been selected from the available alternatives, we might want to reintroduce the design variables and cost functions that were eliminated for the screening optimizations. Of course, we could use the same concepts developed above to determine the optimum design. For example, we can define trade-off functions as the sum of all cost functions that contribute to the increasing or decreasing cost gradients for each design variable. Thus, the trade-off functions for the reactor conversion in our example are given by

$$F_x^+ = \frac{\partial}{\partial x}(f_1 + f_2 + f_3 + f_9 + f_{10} + f_{11} + f_{12} + f_{13})$$

$$F_x^- = \frac{\partial}{\partial x}(f_4 + f_5 + f_6 + f_7 + f_8) \quad (15)$$

Then, the necessary condition for the optimum conversion is that

$$F_x^+ = -F_x^- \quad (16)$$

which is equivalent to the condition that the gradient ($\partial TAC/\partial x$) is equal to zero. Similar cost functions for the remaining variables can be developed by noting the cost gradients in Table 2.

We can again use r_j to establish a rank-order of optimization variables. Variables with r_j's of similar order of magnitude might then be rank-ordered with decreasing values of p_j. Optimizing the variables according to this hierarchy and iterating might lead to reduced computing times for large problems.

We could still use p_j as a criterion for optimality for this problem, although a stricter criterion might be implemented (e.g., $p_j < 0.1$ or 0.2 for each x_j). Moreover, we might consider using stricter criteria for the most important design variables. Again, we note that it is not prudent to make these criteria so strict that we exceed the accuracy of the design and economic models being implemented.

OPTIMUM STEADY-STATE CONTROL ANALYSIS

Once the design of each piece of equipment in a flowsheet is specified, the nature of the process optimization is changed in three ways:

1. Specification of equipment sizes reduces the number of degrees of freedom for the process. Thus the number of control optimization variables is considerably smaller than the number of design optimization variables.
2. The capital costs are eliminated from the problem formulation. Thus the economic trade-offs for the remaining variables are quite different from those at the design stage.
3. The new optimum flows for steady-state control (i.e., the flows which minimize the operating costs for the process) often cannot be attained with equipment sizes fixed for optimum design conditions. Thus the control optimization problem is often constrained.

For the simple reaction system $A \rightarrow P \rightarrow W$ described above, specification of the reactor volume and the number of trays in the product column reduces the number of optimization variables to two. If we consider these variables to be the reactor conversion and the reflux ratio for the product column, we can reevaluate the process economic trade-offs for each. The reflux ratio, for example, trades off poor recovery of the product overhead (for constant product composition) at low reflux ratios vs. high steam and cooling water costs at high reflux ratios.

At the design stage, the flow optimization variables generally trade off capital vs. operating costs for equipment in the liquid and/or gas recycle loops. Once the equipment sizes are fixed, however, these optimizations can only trade off operating costs. Thus, we should not expect that the unconstrained optimum flows for steady-state control will be equal to those at the design stage. Unfortunately, realizing these new optimum flows would normally require excessive overdesign policies to prevent saturation of the equipment in the recycle loops.

If the equipment sizes correspond exactly to the optimum design values (i.e., with no overdesign) and if no disturbances are present (i.e., the operating conditions equal the assumed base-case design conditions), the constrained optimum flows would correspond exactly to the optimum design values. However, some overdesign policy must be implemented in order to insure operability of the process in the face of disturbances. For this case, the constrained optimum flows may not be identical to those at the design stage, even if no disturbances are present. Obviously, the equipment overdesign factors selected will have a significant effect on the results of the optimization analysis, affecting both the operating and capital costs for the process.

The rank-order and proximity parameters defined for the design optimization formulation are of only limited utility for the control problem. The rank-order parameter can still be used to determine the relative importance of the control optimization variables. However, if important variables are always constrained, these optimizations have trivial solutions. Moreover, the proximity parameter still approaches zero as the variables reaches its unconstrained optimum, but it is meaningless for constrained optimization variables. Nonetheless, understanding the change in the nature of the optimization problem for the steady-state control problem is useful for studying steady-state control based on the process economics. Fisher et al. (1984) have applied this approach to a complete chemical plant.

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NOTATION

A	= heat exchanger area
C	= equipment capital cost
E	= activation energy
F	= flowrate
f	= fractional recovery
F_j^+, F_j^-	= sum of all cost functions contributing to the positive or negative gradient for design variable x_j
f_i	= annualized cost function
G	= vapor flowrate in a gas absorber
k	= reaction rate constant
K_1	= K factor for a heavy component in a flash drum feed stream
L	= solvent flowrate in a gas absorber
m	= slope of the equilibrium line in a gas absorber
N	= number of trays
P	= production rate
p_j	= proximity parameter for design variable x_j
R	= reflux ratio
r_j	= rank-order parameter for design variable x_j
S	= selectivity
T	= temperature, K
ΔT	= heat exchanger approach temperature
ΔT_m	= log-mean temperature driving force
Δt	= temperature change for a process stream through an exchanger
TAC	= total annualized cost
U	= heat transfer coefficient
V	= column vapor flowrate
V_R	= reactor volume
x	= reactor conversion for component A
x_j	= optimization variable

Greek Letters

α	= relative volatility
β	= correction factor, see Eq. A18
ρ	= density

Subscripts

A	= component A (reactant)
BC	= base-case
comp	= compressor
cond	= condenser
cw	= cooling water
F	= feed stream
FA	= fresh feed of component A
furn	= furnace
P	= component P (product)
R	= reactor
reb	= reboiler
sh	= shell
W	= component W (waste)

APPENDIX A: CAPITAL COST MODELS FOR SEVERAL EQUIPMENT TYPES

Isothermal Plug Flow Reactors. For a first-order isothermal reaction in a tubular reactor, the design equation is

$$V_R = \frac{F}{k\rho} \ln\left(\frac{1}{1-x}\right) \quad \text{(A1)}$$

The installed cost of this reactor can be written as

$$C_R = C_{R,BC}\left(\frac{V_R}{V_{R,BC}}\right)^{0.63} \quad \text{(A2)}$$

We can relate the cost of the reactor for any conversion to the cost of the reactor at base-case conditions as follows

$$C_R = C_{R,BC}\left[\frac{F \ln(1-x) k_{BC}}{F_{BC} \ln(1-x_{BC}) k}\right]^{0.63} \quad \text{(A3)}$$

Furnaces. Available cost models for direct-fired heaters relate the installed cost to the furnace heat duty only, for example

$$C_F = C_{F,BC}\left(\frac{Q_F}{Q_{F,BC}}\right)^{0.78} \quad \text{(A4)}$$

The (sensible) heat duty for the furnace is

$$Q_F = FC_P\Delta t \quad \text{(A5)}$$

so that our cost model becomes

$$C_F = \left(\frac{F\Delta t}{F_{BC}\Delta t_{BC}}\right)^{0.78} \quad \text{(A6)}$$

Compressors. The installed cost for a compressor can be related to the required brake horsepower (Bhp = Power/efficiency)

$$C_{\text{comp}} = C_{\text{comp},BC}\left(\frac{Bhp}{Bhp,Bc}\right)^{0.93} \quad \text{(A7)}$$

The power required for isentropic compression of an ideal gas stream is

$$\text{Power} = 3.03 \times 10^{-5}\left(\frac{k}{k-1}\right) p_{\text{in}} F_v \left[\left(\frac{p_{\text{in}}}{p_{\text{out}}}\right)^{(k-1/k)} - 1\right] \quad \text{(A8)}$$

where:

$$k = C_P/C_V \quad \text{(A9)}$$

If the gas composition is constant and the inlet and outlet pressures are roughly constant for a fixed flowsheet, then the cost model becomes

$$C_{\text{comp}} = C_{\text{comp},BC}\left(\frac{F_v}{F_{v,BC}}\right)^{0.93} \quad \text{(A10)}$$

For gas recycle compressors, both the vapor flowrate and composition may vary (if purge composition is optimized). In this case, the ratio of heat capacities, k, may also be included in the cost model.

Distillation Columns. The installed cost of a distillation column shell (with trays or packing) can be written as

$$C_{\text{sh}} = C_{\text{sh},BC}\left(\frac{N}{N_{BC}}\right)^{0.802}\left(\frac{\text{Dia}}{\text{Dia}_{BC}}\right)^{1.066} \quad \text{(A11)}$$

The column diameter varies as the square root of the column vapor rate, so we can write

$$C_{\text{sh}} = C_{\text{sh},BC}\left(\frac{N}{N_{BC}}\right)^{0.802}\left(\frac{V}{V_{BC}}\right)^{0.533} \quad \text{(A12)}$$

The vapor rate in the column is given by

$$V = (R+1)D \quad \text{(A13)}$$

For reasonably sharp splits, the distillate flowrate is approximately $x_F F$. If the outlet composition and reflux ratio are not optimized, the number of trays for the required separation is essentially constant. For this case, our model becomes

$$C_{\text{sh}} = C_{\text{sh},BC}\left\{\frac{(1.2R_m + 1)x_F F}{[(1.2R_m + 1)x_F F]_{BC}}\right\}^{0.533} \quad \text{(A14)}$$

If the outlet compositions are optimized, but the reflux ratio is fixed (at, say, 1.2 times the minimum), the cost model is

$$C_{sh} = C_{sh,BC}\left(\frac{\ln S}{\ln S_{BC}}\right)^{0.802}\left(\frac{V}{V_{BC}}\right)^{0.533} \quad (A15)$$

where:

$$S = \left(\frac{x_D}{1-x_D}\right)\left(\frac{1-x_B}{x_B}\right) \quad (A16)$$

If we also wish to optimize the reflux ratio, we can use the approximate design model of Jafarey et al. (1979)

$$N = \frac{\ln \beta S}{\ln\left\{\alpha \Big/ \left[1+\frac{R/R_m}{\alpha-1}\right]^{0.5}\right\}} \quad (A17)$$

where:

$$\beta = \frac{[(R/R_m - 1) + \alpha x_F](R/R_m - x_F)}{(R/R_m - 1)^2} \quad (A18)$$

The installed cost of the column reboiler and condenser can be written as

$$C_R = C_{R,BC}\left(\frac{A_R}{A_{R,BC}}\right)^{0.65} = C_{R,BC}\left(\frac{V}{V_{BC}}\right)^{0.65} \quad (A19)$$

$$C_C = C_{C,BC}\left(\frac{A_C}{A_{C,BC}}\right)^{0.65} = C_{C,BC}\left(\frac{V}{V_{BC}}\right)^{0.65} \quad (A20)$$

Similarly, the operating costs for steam and cooling water can be written as

$$C_{stm} = C_{stm,BC}\left(\frac{V}{V_{BC}}\right) \quad (A21)$$

$$C_{cw} = C_{cw,BC}\left(\frac{V}{V_{BC}}\right) \quad (A22)$$

APPENDIX B: DEVELOPMENT OF AN ECONOMIC MODEL FOR EXAMPLE REACTOR SYSTEM

Process Flows and Stream Costs

The flowsheet for the simple reaction system $A \rightarrow P \rightarrow W$ was given in Figure 1. We assume that a feed stream containing pure A is available and that all A fed to the process is recycled to extinction. That is, we assume a perfect split between A and P in the recycle column (although this assumption will be relaxed for the actual column design below). The overall material balance for the process is given by

$$F_{FA} = P + W \quad (B1)$$

The product flowrate, P, is fixed, as well as the product stream composition

$$x_{D,P} = P_P/P = 0.999 \quad (B2)$$

The fractional recovery of P in the product column is given by

$$f_P = \left(\frac{P_P}{P_P + W_P}\right) \quad (B3)$$

We define the selectivity of the reaction system

$$S = \left(\frac{\text{moles of } P \text{ in reactor outlet}}{\text{moles of } A \text{ converted}}\right) \quad (B4)$$

$$= \frac{P_P + W_P}{P + W} \quad (B5)$$

The raw material cost for the process is

$$\text{Feed} = C_F F_{FA} = (\$15.5/\text{mol})\left(8{,}150\,\frac{\text{hr}}{\text{yr}}\right)\left(\frac{P x_{D,P}}{f_P S}\right) \quad (B6)$$

Of course, when we calculate the annual processing costs we want to subtract the cost of the feed which corresponds to the stoichiometric minimum. We assume the by-product value of the waste stream is

$$\text{By-product} = C_W W = (\$1.0/\text{mol})\left(8{,}150\,\frac{\text{hr}}{\text{yr}}\right)\left(\frac{x_{D,P}}{f_P S} - 1\right)P \quad (B7)$$

The value of the primary product is

$$\text{Product} = C_P P = (\$20.0/\text{mol})P \quad (B8)$$

Equipment Cost Models

Reactor. The kinetic model for the reaction system is assumed to be

$$dC_A/dt = -k_1 C_A$$
$$dC_P/dt = k_1 C_A - k_2 C_P \quad (B9)$$

$$k_1 = 5.35 \times 10^{10} \exp\left(\frac{-9{,}050}{T}\right) \text{min}^{-1}$$
$$k_2 = 4.61 \times 10^{17} \exp\left(\frac{-15{,}100}{T}\right) \text{min}^{-1} \quad (B10)$$

For an isothemal plug flow reactor system, the reactor volume is given by

$$V_R = \left(\frac{F}{k_1 \rho}\right) \ln\left(\frac{1}{1-x}\right) \quad (B11)$$

where x is the extent of conversion of A and the total reactor feed flowrate is

$$F = F_{FA}/x \quad (B12)$$

Our simplified reactor cost model is then

$$C_R = C_{R,BC}\left(\frac{V_R}{V_{R,BC}}\right)^{0.63} \quad (B13)$$

Also, we can calculate the selectivity as a function of reactor temperature and conversion (our assumed design variables)

$$S = \left(\frac{1}{x}\right)\left[\frac{1}{1-k_1/k_2}\right][(1-x)^{k_1/k_2} - (1-x)] \quad (B14)$$

Recycle Column. We are not interested in optimizing the design of the recycle column in this case study, but we want to include its cost in the economic model. We assume that the design reflux ratio is 1.2 times the minimum, for which the theoretical number of trays is about twice the minimum. That is

$$N = 2N_m = 2\,\frac{\ln S}{\ln \alpha_{AP}} \quad (B15)$$

An approximate expression for the minimum reflux ratio is given by Glinos and Malone (1984):

$$R_m = \left(\frac{\alpha_{PW}}{\alpha_{AW} - \alpha_{PW}}\right)\left(\frac{x_{F,A} + x_{F,P}}{x_{F,A}}\right) + \frac{x_{F,W}}{x_{F,A}(\alpha_{AW} - 1)} \quad (B16)$$

where:

$$x_{F,A} = 1 - x$$
$$x_{F,P} = xS$$
$$x_{F,W} = (1 - S)x$$

From Appendix A, the appropriate cost model for this case is

$$C_{sh1} = C_{sh1,BC}\left(\frac{V_1}{V_{1,BC}}\right)^{0.533} \quad (B17)$$

The column vapor rate is calculated by

$$V_1 = (1.2R_m + 1)D$$

$$= (1.2R_m + 1)\left[\frac{(1-x)F_{FA}}{x}\right] \tag{B18}$$

The recycle column condenser and reboiler capital costs are given by

$$C_{C1} = C_{C1,BC}(V_1/V_{1,BC})^{0.65} \tag{B19}$$

$$C_{R1} = C_{R1,BC}(V_1/V_{1,BC})^{0.65} \tag{B20}$$

The associated operating costs are, for cooling water and steam,

$$C_{cw1} = C_{cw1,BC}(V_1/V_{1,BC}) \tag{B21}$$

$$C_{stm1} = C_{stm1,BC}(V_1/V_{1,BC}) \tag{B22}$$

Product Column. The desired economic model for the product column shell is also of the form

$$C_{sh2} = C_{sh2,BC}(N/N_{BC})^{0.802}(V_2/V_{2,BC})^{0.533} \tag{B23}$$

In this case, we could use the design model of Jafarey et al. (1979) to allow optimization of the design reflux ratio and the product recovery fraction (see Eq. A17). The distillate composition is fixed and the bottoms composition is calculated from

$$x_{B,P} = \frac{(1-f_P)x_{D,P}S}{x_{D,P} - f_P S} \tag{B24}$$

and the vapor rate from

$$V_2 = (R + 1)D_2$$

$$= \left[\frac{R/R_m}{(\alpha_{PW} - 1)S} + 1\right]P \tag{B25}$$

The condenser, reboiler, cooling water, and steam costs are given by

$$C_{C2} = C_{C2,BC}(V_2/V_{2,BC})^{0.65} \tag{B26}$$

$$C_{R2} = C_{R2,BC}(V_2/V_{2,BC})^{0.65} \tag{B27}$$

$$C_{cw2} = C_{cw2,BC}(V_2/V_{2,BC}) \tag{B28}$$

$$C_{stm2} = C_{stm2,BC}(V_2/V_{2,BC}) \tag{B29}$$

Summary

The annualized cost expressions for this process have been simplified and are presented in Table 1. The cost functions are developed using the base-case conditions $x = 0.8$, $T_{rxn} = 305$ K, $f_P = 0.995$, and $R = 1.2R_m$.

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