Design for Operability: A Singular-Value Optimization Approach within a Multiple-Objective Framework

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Design-for-operability is a field of active research in process systems engineering because of the high economic impact of design on operability. Dynamic operability has been widely studied by means of the so-called (open-loop) controllability and resiliency indices, which are mostly based on linearized (Laplace/frequency domains) models of the dynamic systems. In particular, the minimum singular value of the transfer function matrix is a fair measure of resilience to disturbances. Among the plethora of approaches to design for dynamic operability, a multiple-objective formulation between cost and controllability naturally arises because of the conflicting characters of the two objectives. In this contribution the cost/minimum-singular-value multiple-objective design problem is solved for the meaningful reactor−separator−recycle system and two different control strategies. The generation of the noninferior solution set is performed here within the framework of an eigenvalue optimization approach.

1. Introduction

Systems design problems can be mathematically formulated as optimization problems, in which a meaningful objective (usually economic) is aimed to be optimized while model constraints (equalities and inequalities) are satisfied.

Certain operability issues should also be considered for proper design. Operability is a broad concept that has to do with the behavioral features of the system. In this work, we focus on the dynamic implications of operability, that is, the appeal of our system in a dynamic sense.

Because dynamic operability features depend on the process itself, rather than, for example, on control strategies, design-for-operability is an active research field in engineering. It is particularly important to chemical engineering because of the economic magnitude of the involved processes.

The work on design-for-operability is quite vast, as it includes the also-large literature on dynamic assessment techniques. In the following discussion, only the major approaches are described. The review in Bansal[1] as well as the works by Morari and Perkins[2] and Lewin[3] are highly recommended for further reading on the subject.

Sequential Approach to Process Design. Process design is evolving toward a completely integrated and automated activity. However, it still requires “artistic” skills from the designer. This is because full nonlinear optimization design/synthesis with convenient closed-loop dynamic behavior under disturbances and parametric uncertainty is a very difficult problem.

Current design/synthesis practice, therefore, involves the proposal of reasonable flowsheets based on engineering criteria and experience and the optimization of single economic objective functions subject to the steady-state model of the proposed processes.

To perform operability assessment, the designs thus generated are classified according to certain operability measures. Such operability measures, better known as controllability and resiliency (C&R) indices, are based on linearized versions of the open-loop nonlinear differential algebraic models of the process and are defined in the frequency domain. These measures include nonminimum phase elements (right-half-plane zeros, right-half-plane poles, and time delays), singular values, condition number, and Relative Gain Array (RGA).

Once the design is deemed satisfactory according to some or all of these measures, it is further developed. This approach has the advantage that poorly operable designs can be discarded early without waste of time and effort.

At this point, an adequate control strategy is proposed, and intense steady-state and dynamic simulations are performed to assess the system behavior in the face of disturbance and parametric uncertainty and set-point changes. In general, open-loop stability is desired, and controller tuning seeks quick and smooth transients. The design is also dynamically evaluated regarding “path constraints” to verify that no state violates possible lower or upper bounds imposed by operational or safety considerations during the transients.

If satisfactory dynamic behavior is not observed, the process flowsheet is improved, or new ones are tried. This procedure is performed repeatedly until a satisfactory design is achieved.

Nonlinear dynamic simulation is, by far, the most widely applied tool for evaluating the dynamic performance of chemical processes. Despite its inherent advantages, mainly the ability to handle large and involved nonlinear systems, extensive dynamic simulation can be time-intensive and computationally expensive at the design stage.

This rather heuristic approach requires a great deal of experience-based knowledge and ingenuity for the early proposal of successful flowsheet alternatives. However, it provides a very intuitive framework for addressing the complex design-for-operability problem, and meaningful contributions have been produced on

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the subject in the past decade, particularly the work by Luyben et al.[4]

Integrated Design and Operability. Process dynamic operability can be considered in mainly two ways within the design problem: through operability (C&R) analysis tools and through dynamic simulations. These strategies give rise to the two major approaches to design-for-operability: multiobjective optimization and dynamic optimization. In the following discussion, these two major approaches to address the design-for-operability problem in an integrated fashion are briefly described.

Multiobjective Optimization Approach. Multiobjective optimization problems arise when it is necessary to consider competing objectives, that is, when one of the objectives can be improved only at the expense of the other(s). This situation is rather common in design, and it is indeed the case in design-for-controllability.

A multiobjective problem can naturally be posed between economic objectives and C&R indices, as proposed by Palazoglu and Arkun[5] and Luyben and Floudas.[6]

Other operability indices have also been considered within such a strategy.[7,8]

The main advantage of using multiobjective optimization to address the design-for-operability problem is that the objectives have very intuitive meanings and the tradeoffs among them can be clearly traced.

The use of linear operability objectives presents, however, several limitations.[9] First, linear approximations might not be reliable enough for the usually highly nonlinear process systems in the face of uncertainty. Some of the measures assume square (Laplace domain) plants, which might be unrealistic. These indices are defined in the frequency domain, whereas the performance requirements are established in the time domain, and the translation might not be straightforward. Finally, the application of these tools requires the use of heuristics and experience to overcome the subjectivity of their definition.

Dynamic Optimization Approach. This approach considers process design and process operability simultaneously as one integrated optimization problem. This is an attractive approach indeed, as both flowsheet synthesis and operability analysis are fully automated.

Process synthesis reduces to the development of a superstructure of process flowsheets, which might include the possible control schemes, introducing binary decision variables within the formulation.

Satisfactory process controllability is ensured because the dynamics of the (closed-loop) system is explicitly considered through the set of differential equations, giving rise to a dynamic optimization problem.

Steady-state and dynamic process feasibility are also ensured because disturbance and parametric uncertainty are explicitly taken into account (through a deterministic or stochastic approach).

The very general formulation results in a mixed integer nonlinear, infinite-dimensional dynamic optimization problem. Different versions of this problem have been addressed by Mohideen et al.,[10] Schewiger and Floudas,[11] and Bansal.[1]

The solution of the full problem is a very complex task, and only simplified versions have been recently solved. First, systematically developing superstructures for process flowsheets is a difficult task. The handling of dynamic behavior and uncertainty in mixed integer nonlinear programming problems is also an involved problem. Finally, this approach involves significant demands on computational resources.

This second integrated approach to design-for-operability presents very attractive features as it allows the explicit consideration of most of the required design issues within a very elegant formulation. The major drawback of such an approach is the inherent difficulty in modeling and solving the resulting complex programming problem.

The multiobjective approach, on the other hand, has a much simpler formulation and solution strategy. It relies on steady-state optimization models and rather intuitive operability objectives if C&R indices are considered. Of course, it suffers the limitations of applying linear tools to study nonlinear dynamic systems as discussed above.

In this work, a multiobjective cost/controllability approach to the design-for-operability problem is considered. Such an approach has been addressed by Luyben and Floudas,[6] among others, as already noted.

In that contribution, the multiobjective strategy was applied, for several C&R measures, to the design of various meaningful chemical engineering processes. Pareto-optimal solutions between cost and a C&R index were generated, and the best compromise solution was evaluated in some way. In particular, minimum-singular-value analytical expressions were supplied to the NLP optimization model as functions of the optimization variables.

The original contribution of this work is the implementation of eigenvalue optimization techniques to deal with the controllability objective, namely, the minimum singular value of the zero-frequency process transfer function matrix, within the multiobjective optimization problem. It is the purpose of this work to introduce the possibilities of eigenvalue optimization to the chemical engineering community and to demonstrate its features through the important design-for-operability problem.

Eigenvalue optimization is an active research discipline in mathematics and engineering, although it is almost unexplored in the chemical engineering field. Alternative applications of eigenvalue optimization to the design-for-operability problem can be found in Blanco and Bandoni.[12]

The proposed formulation is applied to the reaction−separation−recycle process, of outstanding importance in chemical engineering.

The paper is outlined as follows. In the next section, the most relevant theoretical topics covered in this paper, namely, singular-value analysis, eigenvalue optimization, and multiobjective optimization, are introduced. Then the model of the reactor−separator−recycle system (taken from Luyben[13]) is described. Finally, the proposed approach is applied to the generation of the nonminimum solution sets of the cost/controllability design problem for two control configurations.

2. Theoretical Framework

2.1. Singular-Value Controllability Analysis. C&R measures, such as singular values, condition number, and RGA, are based on linearized versions of multiple-input/multiple-output dynamic models in the Laplace and frequency domains

$$\mathbf{y}(s) = \mathbf{G}(s)\,\mathbf{u}(s) + \mathbf{G_d}(s)\,\mathbf{d}(s)$$

In particular, the minimum singular value of the steady-state (zero-frequency) transfer function matrix, $\mathbf{G}$

$$\sigma_{\min}(\mathbf{G}) = \min_{||\mathbf{u}||\neq 0} \frac{||\mathbf{G}\mathbf{u}||_2}{||\mathbf{u}||_2}$$

indicates how close this matrix is to being singular and represents the smallest gain of the process among possible input directions. A large value of this measure implies that the process is resilient to disturbances. The singular values of matrix **G** can be calculated as the square roots of the eigenvalues of $\mathbf{H} = \mathbf{G}^{\mathrm{T}}\mathbf{G}$

$$\sigma_i(\mathbf{G}) = \sqrt{\lambda_i(\mathbf{H})} \qquad i = 1, ..., n$$

Specifically

$$\sigma_{\min}(\mathbf{G}) = \sqrt{\lambda_{\min}(\mathbf{H})}$$

Another meaningful index, which is introduced to provide a most complete description of the controllability theory, is the condition number of matrix **G**, defined as

$$\gamma(\mathbf{G}) = \frac{\sigma_{\max}(\mathbf{G})}{\sigma_{\min}(\mathbf{G})}$$

which verifies the following relation

$$\frac{||\delta\mathbf{u}||}{||\mathbf{u}||} = \gamma(\mathbf{G})\frac{||\delta\mathbf{G}||}{||\mathbf{G}||}$$

A small condition number means that model errors do not cause large errors in the manipulated variable.

As discussed by Luyben and Floudas,[6] controllability measures can be calculated not only at steady state but also as functions of frequency so that dynamics can be considered. We limit ourselves here to a steady-state analysis because of inherent difficulties in considering frequency dependence. Frequency-dependent controllability, however, has been studied within a multiobjective approach by Palazoglu and Arkun,[5] for example.

In previous approaches (e.g., Luyben and Floudas[6]), explicit analytical expressions for singular values were supplied and straightforwardly incorporated into the design model within a multiobjective optimization framework, as already described. In this work, a different technique, which makes use of eigenvalue optimization ideas, is applied.

2.2. Eigenvalue Optimization. It is impossible to obtain explicit mathematical expressions for the eigenvalues of systems larger than 4 × 4. This makes it impossible to include eigenvalues within the optimization model in a straightforward manner (as objectives and/or constraints). Furthermore, even in the cases where analytical expressions can be obtained, their typical high complexity and nonconvexity make them difficult for standard NLP solvers to handle.

Moreover, a critical difficulty in eigenvalue optimization problems is the potential coalescence of eigenvalues. The eigenvalues of a matrix with differentiable elements (smooth in the optimization variables) are themselves nondifferentiable (nonsmooth) at the points where coalescence occurs. Also, frequently, the optimization objective tends to make the eigenvalues coalesce at the solutions. See Blanco and Bandoni[12] for further references on the subject.

To overcome such difficulties, it is necessary to develop specialized optimization methods when eigenvalues are present. In the following, an eigenvalue optimization strategy for symmetric matrices is introduced and applied to the singular-value optimization problem.

Because singular values are defined in terms of the eigenvalues of the symmetric matrix **H**, a fairly straightforward implementation of singular-value optimization within multiobjective design is possible.

Consider the maximization of the smallest eigenvalue of a symmetric matrix **H**(**y**)

$$\begin{aligned} &\max_{\mathbf{y}} \lambda_{\min}[\mathbf{H}(\mathbf{y})] \\ \text{s.t.}\quad &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \end{aligned}$$

This problem can be reformulated in terms of the auxiliary variable z (Ringertz[14]). The strategy is to bound the spectrum from below and maximize the lower bound z

$$\begin{aligned} &\max_{\mathbf{y},z} z \\ \text{s.t.}\quad &\lambda_i[\mathbf{H}(\mathbf{y})] \geq z \qquad i = 1, ..., n \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \\ &z^{\mathrm{l}} \leq z \end{aligned}$$

Because $\mathbf{H}\cdot\mathbf{v} = \lambda\mathbf{I}\cdot\mathbf{v}$ implies $(\mathbf{H} - z\mathbf{I})\cdot\mathbf{v} = (\lambda - z)\mathbf{I}\cdot\mathbf{v}$, the condition $\lambda_i - z > 0$ implies that $\mathbf{H} - z\mathbf{I} > \mathbf{0}$. Here, $> \mathbf{0}$ indicates positive definiteness. Therefore, the above problem can be rewritten as

$$\begin{aligned} &\max_{\mathbf{y},z} z \\ \text{s.t.}\quad &\mathbf{H}(\mathbf{y}) - z\mathbf{I} > \mathbf{0} \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \\ &z^{\mathrm{l}} \leq z \end{aligned}$$

Several approaches have been proposed to solve the above problem.[12,14]

In this work, positive definiteness of symmetric matrix $\mathbf{H} - z\mathbf{I}$ is ensured through Sylvester's criterion, which states that the necessary and sufficient conditions for a symmetric matrix $\mathbf{A}(n,n)$ to be positive-definite are that its successive principal minors $\mathbf{A}_i$ ($i = 1, ..., n$) be positive: det[$\mathbf{A}(1,1)$], det[$\mathbf{A}(2,2)$], ..., det[$\mathbf{A}(n,n)$].

$$\begin{aligned} &\max_{\mathbf{y},z} z \\ \text{s.t.}\quad &\det\{[\mathbf{H}(\mathbf{y}) - z\mathbf{I}]_i\} > \xi \qquad i = 1, ..., n \\ &\xi > 0 \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \\ &z^{\mathrm{l}} \leq z \end{aligned} \tag{1}$$

This is an NLP problem, which can be solved with standard nonlinear optimization solvers.

ξ is a small positive parameter that is arbitrarily chosen. It was set to 1×10^{-5} in the examples considered.

In a similar fashion, it is possible to formulate the minimization of the maximum eigenvalue of symmetric matrix $\mathbf{H}(\mathbf{y})$ by bounding its spectrum from above with an auxiliary variable z and minimizing this upper bound.

By performing operations analogous to those used in the maximization problem, one obtains

$$\begin{aligned} &\min_{\mathbf{y},z} z \\ \text{s.t.}\quad &\det\{[z\mathbf{I} - \mathbf{H}(\mathbf{y})]_i\} > \xi \qquad i = 1, ..., n \\ &\xi > 0 \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \le \mathbf{0} \\ &\mathbf{y} \in Y \\ &z \le z^{\mathrm{u}} \end{aligned} \tag{2}$$

In the following example, a very simple singular-value optimization problem is solved to illustrate the described ideas. The purpose of this example of intuitive meaning is to show that the proposed optimization strategies produce the desired results regarding the singular-value structure of the matrix.

Consider the following classic example used to introduce matrix singularity theory

$$\mathbf{B}(\epsilon) = \begin{bmatrix} 1 & 0 \\ 1/\epsilon & 1 \end{bmatrix}$$

This pathological matrix is often used to show how poor the determinant is as an indicator for studying singularity.[15] Even though the determinant of $\mathbf{B}(\epsilon)$ is always equal to 1, $\mathbf{B}(\epsilon)$ approaches singularity as ϵ becomes smaller.

According to the above explanation, the problem of maximizing the minimum singular value of matrix $\mathbf{B}(\epsilon)$

$$\begin{aligned} &\max_{\epsilon} \lambda_{\min}[\mathbf{B}(\epsilon)^{\mathrm{T}}\cdot\mathbf{B}(\epsilon)] \\ \text{s.t.}\quad &\epsilon^{\mathrm{l}} \le \epsilon \le \epsilon^{\mathrm{u}} \end{aligned}$$

can be posed according to eq 1 as

$$\begin{aligned} &\max_{\epsilon,z} z \\ \text{s.t.}\quad &\det\{[\mathbf{B}(\epsilon)^{\mathrm{T}}\cdot\mathbf{B}(\epsilon) - z\mathbf{I}]_i\} > \xi \qquad i = 1, 2 \\ &\xi > 0 \\ &\epsilon^{\mathrm{l}} \le \epsilon \le \epsilon^{\mathrm{u}} \end{aligned}$$

where

$$\mathbf{B}(\epsilon)^{\mathrm{T}}\cdot\mathbf{B}(\epsilon) = \begin{bmatrix} 1 + (1/\epsilon)^2 & 1/\epsilon \\ 1/\epsilon & 1 \end{bmatrix}$$

As expected, the solution of this problem corresponds to $\epsilon = \epsilon^{\mathrm{u}}$, and $z \to 1$, $\sigma_1 \to 1$, and $\sigma_2 \to 1$ as $\epsilon^{\mathrm{u}} \to \infty$.

The same result is obtained if minimization problem 2 is considered.

By combining formulations 1 and 2, it is also possible to formulate alternative problems to consider the condition number of matrix $\mathbf{G}$ by adding upper bounds on the maximum eigenvalue of matrix $\mathbf{H}$

$$\begin{aligned} &\max_{\mathbf{y},z} z \\ \text{s.t.}\quad &\det\{[\mathbf{H}(\mathbf{y}) - z\mathbf{I}]_i\} > \xi \qquad i = 1, ..., n \\ &\det\{[k^{\mathrm{u}}\mathbf{I} - \mathbf{H}(\mathbf{y})]_i\} > \xi \qquad i = 1, ..., n \\ &\xi > 0 \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \le \mathbf{0} \\ &\mathbf{y} \in Y \\ &z \le z^{\mathrm{u}} \end{aligned}$$

In the above formulation, k^{u} is chosen to be an upper bound of the maximum eigenvalue of matrix $\mathbf{H}$. Because the square of the condition number of matrix $\mathbf{G}$ is the ratio between the maximum and minimum eigenvalues of matrix $\mathbf{H}$, the following constraint on the condition number can be straightforwardly included: $\gamma^2(\mathbf{G}) \le k^{\mathrm{u}}/z$.

The proposed eigenvalue optimization approach provides a systematic framework to handle the whole spectrum of even medium- and large-scale symmetric matrices by bounding both minimum and maximum eigenvalues. In Blanco and Bandoni,[12] similar ideas are applied to handle the spectrum of unsymmetric matrices.

2.3. Multiobjective Optimization. Common practice in multiobjective optimization is to generate the noninferior solution set in some way and then select among its members according to a certain decision maker's preference.

The expected qualitatively noninferior solution set for the cost/minimum-singular-value problem is roughly depicted in Figure 1.

To generate the noninferior solution set, the classic ϵ-constraint method is applied here between the cost and the minimum singular value of the transfer function matrix of the process.

The idea is to maximize variable z (which bounds from below the spectrum of $\mathbf{H}$ and, therefore, the minimum singular value of matrix $\mathbf{G}$) as in eq 1, including an additional constraint on the cost of the process

$$\begin{aligned} &\max_{\mathbf{y},z} z \\ \text{s.t.}\quad &\det\{[\mathbf{H}(\mathbf{y}) - z\mathbf{I}]_i\} > \xi \qquad i = 1, ..., n \\ &\xi > 0 \\ &\text{cost} \le \epsilon_j \qquad j = 1, ..., p \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \le \mathbf{0} \\ &\mathbf{y} \in Y \\ &z^{\mathrm{l}} \le z \end{aligned}$$

By progressively increasing the value ϵ, different results for the minimum singular value are obtained (the constraint on the cost should be binding at the solution), to calculate the Pareto-optimal solution.

3. Reactor–Separator–Recycle System Model

Chemical plants used to be cascades of individual units. The key for successful dynamic operation of such plants was proper control of each unit.

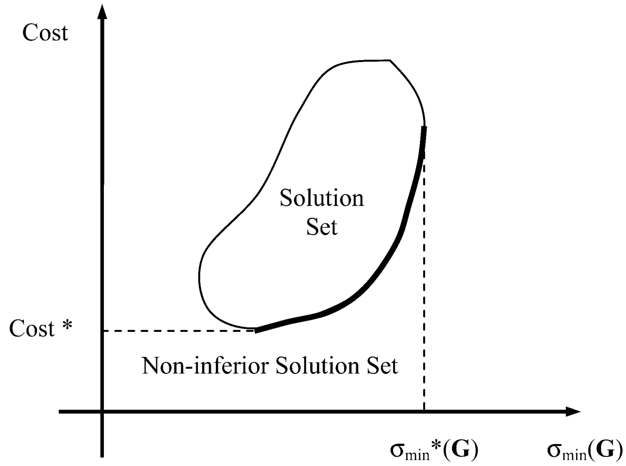

Figure 1. Noninferior solution set for cost and $\sigma_{\min}(\mathbf{G})$.

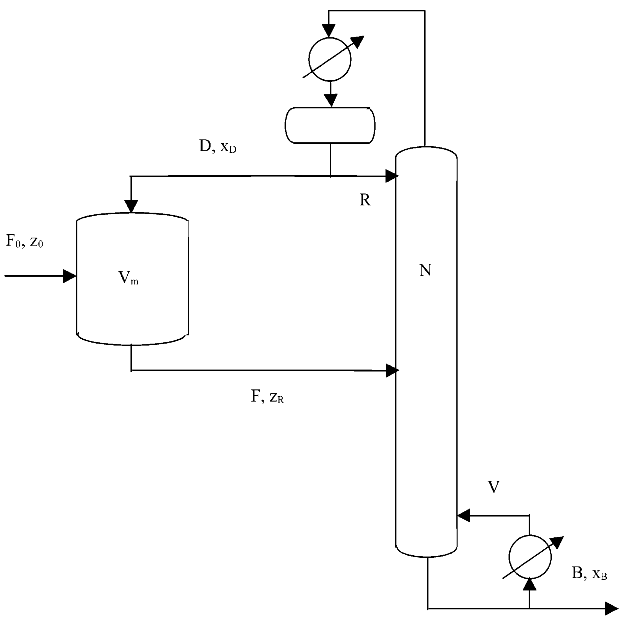

Figure 2. Reactor–separator–recycle system.

Modern chemical plants, on the other hand, are highly integrated (mass and energy recycles) to maximize conversion throughout the whole process and accomplish efficient energetic operation. Integrated plants present complex dynamic behavior because of the positive feedback introduced by the recycles.

Conventional wisdom for handling such complex dynamics is to isolate units by means of large surge tanks, so that dynamic interactions can be reduced. This practice, however, is expensive and can be environmentally unacceptable when hazardous chemicals are involved.

The challenge is therefore to design for the feasible operation of tightly integrated processes. Recycle systems gave rise to the concept of plantwide control, which considers processes as a whole, rather than cascades of units, for control purposes.[4]

In this section, a multiobjective approach between cost and controllability is applied to the design of the outstanding reactor–separator–mass-recycle system. The model considered is taken in full from Luyben.[13] The basic flowsheet of the single-reactor/single-column system is shown in Figure 2.

A first-order A → B reaction takes place in the isothermal reactor. The reactor effluent is fed to a column where nonreacted A and product B are separated. Nonreacted A is recycled back to the reactor.

For a given fresh-feed flow rate, F_0, and composition, z_0, and a certain product specification, x_B, the goal is to calculate the design variables that optimize the two conflicting objectives: cost and controllability.

The optimization variables are the feed flow rate, F, and composition, z_R, to the column; the number of trays, N; the vapor boil-up, V; the reflux flow rate, R; the reflux ratio, RR; the recycle flow rate, D, and composition, x_D; and the reactor hold-up, V_m.

The usual simplifying assumptions are considered in the column model: constant relative volatility between components throughout the whole separation, equimolar overflow, total condenser, partial reboiler, and saturated liquid feed.

The following equations describe the mathematical model for this process. For further details, see Luyben.[13]

3.1. Process Model. Total balance around the reactor

$$F_0 + D = F$$

Component balance around the reactor

$$F_0 z_0 + D x_D = F z_R + V_m k z_R$$

Component balance around the column

$$F z_R = D x_D + B x_B$$

Eduljee design equation

$$\left(\frac{N - N_m}{N + 1}\right) = 0.75\left[1 - \left(\frac{RR - RR_m}{RR + 1}\right)^{0.5668}\right]$$

Minimum reflux ratio

$$RR_m = \frac{1}{\alpha - 1}\left[\frac{x_D}{z_R} - \frac{\alpha(1 - x_D)}{(1 - z_R)}\right]$$

Minimum number of stages

$$N_m = \frac{\ln\left(\frac{x_D}{1 - x_D}\frac{1 - x_B}{x_B}\right)}{\ln \alpha}$$

Reflux ratio

$$RR = \frac{R}{D}$$

Condenser balance

$$V = R + D$$

Applicability of the Eduljee design equation

$$RR \geq 1.0101 RR_m + 0.0101$$

This model has 3 degrees of freedom because it involves 11 equality constraints and 8 variables. From the overall balance, one can immediately see that $F_0 = B$. α stands for the relative volatility.

3.2. Economic Objective. The economic objective is the total cost to be minimized, which includes both capital and utility costs

$$\text{cost} = \frac{1}{\beta_{\text{pay}}}(C_{\text{reactor}} + C_{\text{column}} + C_{\text{exchangers}}) + \beta_{\text{tax}}(C_{\text{utilities}})$$

where β_{pay} is the payback period and β_{tax} is the tax factor. All of the costs involved are in units of dollars per year.

$C_{\text{utilities}}$ mainly corresponds to the hot utility at the reboiler of the distillation column and is calculated as

$$C_{\text{utilities}} = 1207V$$

where V is supplied in kilomoles per hour.

The capital cost of the reactor depends on its size and is calculated here as

$$C_{\text{reactor}} = 17\,639(D_{\text{R}})^{1.066}(2D_{\text{R}})^{0.802}$$

where

$$D_{\text{R}} = 0.3967(0.6366V_{\text{m}})^{1/3}$$

These equations assume that the height of the reactor is twice the diameter. D_{R} is in meters, and V_{m} is in kilomoles.

The capital cost of the column depends on the diameter, D_{C}, and the number of trays, N, according to the equation

$$C_{\text{column}} = 6802(D_{\text{C}})^{1.066}(2.4N)^{0.082} + 548.8(D_{\text{C}})^{1.55}N$$

The diameter affects on the vapor velocity in the column, which is related to the vapor boil-up. It then follows that

$$D_{\text{C}} = 0.0832\sqrt{V}$$

The capital cost of the heat exchangers depends on the areas of the reboiler, A_{R}, and the condenser, A_{C}, which are, in turn, related to the vapor boil-up

$$C_{\text{exchangers}} = 8701A_{\text{R}}^{0.65} + 8701A_{\text{C}}^{0.65}$$

where

$$A_{\text{R}} = 0.512V \qquad A_{\text{C}} = 0.854V$$

The areas are in square meters, and V is again in kilomoles per hour.

3.3. Steady-State Gains. To construct matrix **G** at zero frequency, the steady-state gains for the desired pairing of controlled and manipulated variables should be provided. In the present work, the compositions x_{D} and x_{B} are considered as the controlled variables, and the flow rates R, D, and V are considered as the manipulated variables.

The following expressions[6] relate the aforementioned compositions to some arbitrary manipulated variable, u, and permit the calculation of the steady-state gains

$$\left(\frac{\partial x_{\text{B}}}{\partial u}\right)\left[\kappa_2 + \kappa_4\kappa_6\frac{B}{V_{\text{m}}k} - (\kappa_1 - \kappa_4\kappa_5)\frac{B}{D}\left(1 + \frac{F}{V_{\text{m}}k}\right)\right] = \kappa_3\frac{\partial \text{RR}}{\partial u} + \frac{(x_{\text{D}} - z_{\text{R}})}{D}(\kappa_1 - \kappa_4\kappa_5)\frac{\partial D}{\partial u} \quad (3)$$

$$\left(\frac{\partial x_{\text{D}}}{\partial u}\right) = \frac{(z_{\text{R}} - x_{\text{D}})}{D}\frac{\partial D}{\partial u} - \frac{B}{D}\left(1 + \frac{F}{V_{\text{m}}k}\right)\frac{\partial x_{\text{B}}}{\partial u} \quad (4)$$

where

$$\kappa_1 = \frac{-1}{(N+1)(\ln \alpha)x_{\text{D}}(1 - x_{\text{D}})}$$

$$\kappa_2 = \frac{1}{(N+1)(\ln \alpha)x_{\text{B}}(1 - x_{\text{B}})}$$

$$\kappa_3 = \frac{0.5668(\text{RR}_{\text{m}} + 1)}{(\text{RR} + 1)(\text{RR} - \text{RR}_{\text{m}})}\left(\frac{N - N_{\text{m}}}{N + 1} - 0.75\right)$$

$$\kappa_4 = \frac{-0.5668}{(\text{RR} - \text{RR}_{\text{m}})}\left(\frac{N - N_{\text{m}}}{N + 1} - 0.75\right)$$

$$\kappa_5 = \frac{1}{(\alpha - 1)}\left(\frac{1}{z_{\text{R}}} + \frac{\alpha}{1 - z_{\text{R}}}\right)$$

$$\kappa_6 = \frac{-1}{(\alpha - 1)}\left(\frac{x_{\text{D}}}{z_{\text{R}}^2} + \frac{\alpha(1 - x_{\text{D}})}{(1 - z_{\text{R}})^2}\right)$$

With these expressions, the steady-state transfer function matrix for certain control configurations can be constructed.

4. Control of Two Compositions

In this section, the proposed multiobjective approach for process design between cost and singular-value-based controllability is applied to two different control configurations.

4.1. *RV* Control Configuration. In this section, a noninferior solution set for the cost/minimum-singular-value multiobjective design problem is generated for the RV control configuration, where the reflux, R, and the vapor boil-up, V, are chosen to control compositions x_{D} and x_{B}. For the sake of simplicity, perfect level control is assumed in the process (reactor, reflux drum, and column base).

The desired process transfer function matrix is

$$\mathbf{G} = \begin{bmatrix} \left(\frac{\partial x_{\text{D}}}{\partial R}\right)_V & \left(\frac{\partial x_{\text{D}}}{\partial V}\right)_R \\ \left(\frac{\partial x_{\text{B}}}{\partial R}\right)_V & \left(\frac{\partial x_{\text{B}}}{\partial V}\right)_R \end{bmatrix}$$

Its elements can be calculated from eqs 3 and 4 and the following relations

$$\left(\frac{\partial \text{RR}}{\partial R}\right)_V = \frac{V}{D^2}, \qquad \left(\frac{\partial \text{RR}}{\partial V}\right)_R = -\frac{R}{D^2}$$

$$\left(\frac{\partial D}{\partial R}\right)_V = -1, \qquad \left(\frac{\partial D}{\partial V}\right)_R = 1$$

Singular values depend on the scaling of the variables for fair comparison.

Here, matrix **G** is scaled as follows

$$\mathbf{G}^{\text{scaled}} = \begin{bmatrix} \bar{F}/(1 - \bar{x}_{\text{D}}) & 0 \\ 0 & \bar{F}/\bar{x}_{\text{B}} \end{bmatrix}\mathbf{G}^{\text{unscaled}}$$

where the overbar denotes the nominal variable value.

The proposed approach was applied to the generation of the noninferior solution set of the reactor–separator–recycle system with the parameters presented in Table 1. The quality specification $x_{\text{D}} \geq 0.90$ is included in the

Table 1. Physical Data for Reactor−Separator−Recycle System

parameter	value	parameter	value
F_0	108.7 kmol/h	β_{pay}	3 years
z_0	0.9	β_{tax}	1
x_B	0.001 05	$\bar{F}$	125 kmol/h
α	2	$\bar{x}_B$	0.001 05
k	0.340 86 h^{-1}		

Table 2. Noninferior Set for *RV* Configuration

N	V_m (kmol)	cost ($/year)	$\sigma_{min}(\mathbf{G})$	$\gamma(\mathbf{G})$
30.84	2964	515 000	142.77	4.62
30.92	2993.06	515 500	144.87	4.62
31	3021.71	516 000	146.96	4.63
31.1	3048.91	516 500	149.02	4.63
31.15	3077.96	517 000	151.07	4.63
31.22	3105.6	517 500	153.11	4.63
31.29	3132.96	518 000	155.13	4.63
31.5	3154.07	518 500	157.13	4.63
31.99	3161.17	519 000	159	4.62
32.46	3167.4	519 500	160.73	4.61

analysis to prevent the optimal solution from having a single stripper column ($R = 0$).

Table 2 contains the complete noninferior solution set for the system under study, which is graphically shown in Figure 3. The condition number of **G** is also reported.

4.2. *DV* Control Configuration. Here, the *DV* control configuration is employed, where the distillate flow rate, D, and the vapor boil-up, V, are chosen to control compositions x_D and x_B. Again, perfect level control is assumed in the process (reactor, reflux drum, and column base).

The desired process transfer function matrix is

$$\mathbf{G} = \begin{bmatrix} \left(\frac{\partial x_D}{\partial D}\right)_V & \left(\frac{\partial x_D}{\partial V}\right)_D \\ \left(\frac{\partial x_B}{\partial D}\right)_V & \left(\frac{\partial x_B}{\partial V}\right)_D \end{bmatrix}$$

whose elements are calculated from eqs 2 and 3 and the following relations

$$\left(\frac{\partial \mathrm{RR}}{\partial D}\right)_V = -\frac{V}{D^2}, \quad \left(\frac{\partial \mathrm{RR}}{\partial V}\right)_D = \frac{1}{D}$$

$$\left(\frac{\partial D}{\partial D}\right)_V = 1, \quad \left(\frac{\partial D}{\partial V}\right)_D = 0$$

The same scaling procedure as for the *RV* configuration is applied. The process parameters are again those of Table 1, and the quality specification $x_D \geq 0.90$ is also included to prevent the optimal solution from having a stripper column ($R = 0$).

The noninferior set for the system is reported in Table 3 and depicted in Figure 4.

In this section, the noninferior solution set for the cost/minimum-singular-value problem for two alternative control configurations of the reactor−separator−recycle system were generated. The final design can be obtained by simply deciding among the set elements, according to the decision maker's preferences.

Regarding the condition number, which is related to robustness to model errors, the *RV* configuration ($\gamma_{RV} \approx 4.62$) is a better control scheme than the *DV* configuration ($\gamma_{DV} \approx 6.05$).

As already noted, however, these analyses are steady state in nature, and the final decision should be supported by closed-loop dynamic simulations for possible disturbance and uncertainty scenarios.

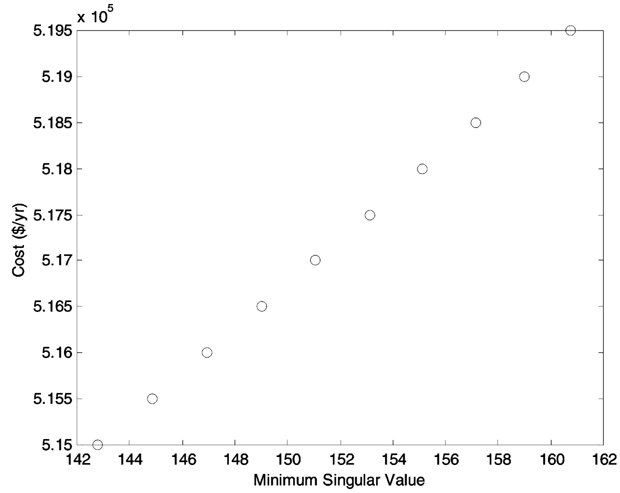

Figure 3. Noninferior solution set for *RV* configuration.

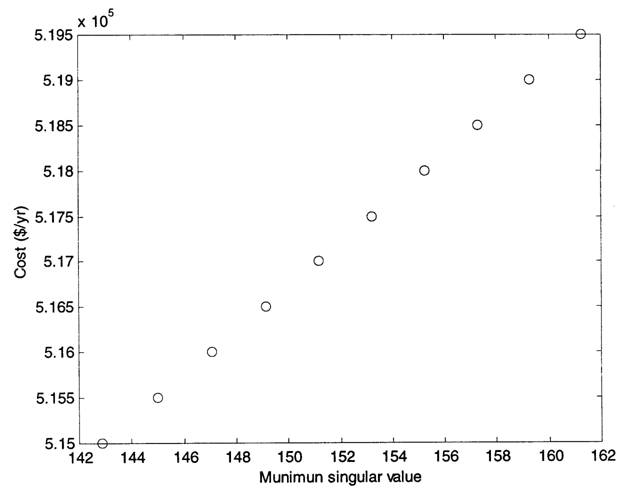

Figure 4. Noninferior solution set for *DV* configuration.

Table 3. Noninferior set for *DV* Configuration

N	V_m (kmol)	cost ($/year)	$\sigma_{min}(\mathbf{G})$	γ (**G**)
30.87	2964.2	515 000	142.9	6.05
30.91	2993.26	515 500	145	6.05
30.99	3021.93	516 000	147.09	6.05
31.07	3050.23	516 500	149.15	6.05
31.14	3078.19	517 000	151.2	6.05
31.21	3105.84	517 500	153.24	6.05
31.29	3133.2	518 000	155.26	6.05
31.36	3160.3	518 500	157.27	6.05
31.43	3187.14	519 000	159.68	6.04
31.5	3213.75	519 500	161.26	6.04

5. Conclusions

Multiobjective optimization is a classic approach to the design-for-operability problem.

In this contribution, a novel strategy to solve the multiobjective cost/controllability design problem has been presented.

The considered controllability index was the minimum singular value of the steady-state process transfer function matrix, which is a fair measure of resilience to disturbances. Because singular values are related to the eigenvalues of symmetric matrices, a direct formulation of the multiobjective problem that makes use of eigenvalue optimization theory was possible.

The proposed optimization scheme was applied to the design of the reactor−separator−recycle system for different control configurations presented in Luyben and Floudas.[6] Noninferior solution sets were generated for each case.

The major advantage of such a formulation is that there is no need to provide explicit expressions for the singular values (eigenvalues), and then large-dimension problems can be tackled in an efficient way.

In fact, the proposed approach provides a systematic framework for handling the whole spectrum of a symmetric matrix by bounding both minimum and maximum eigenvalues. It is therefore possible to formulate alternative problems to consider the condition number of the matrix by adding upper bounds on its maximum eigenvalue.

Although condition numbers and singular values are classic tools for controllability analysis, other open-loop C&R indices, such as RGA and disturbance condition number, exist that should be considered for proper operability assessment. Those that are defined in terms of eigenvalues of symmetric matrices can be handled as described in this work. Others can be considered as regular constraints within the NLP formulation as usual.

Nomenclature

A_C, A_R = heat-exchanger areas for the condenser and reboiler
B = bottoms flow rate
C_{column} = capital cost of the column
$C_{exchangers}$ = capital cost of the exchangers
$C_{reactor}$ = capital cost of the reactor
$C_{utilities}$ = utility cost
D = distillate flow rate
D_C = diameter of the column
D_R = diameter of the reactor
F = feed flow rate to the column
F_0 = fresh-feed flow rate to the reactor
$\mathbf{G}$ = process gain matrix
H_R = reactor height
k = kinetic rate constant
N = number of stages in the column
N_m = minimum number of stages in the column
R = reflux flow rate
RR = reflux ratio in the column
RR_m = minimum reflux ratio
V = vapor boil-up in the column
V_m = molar hold-up in the reactor
x_B, x_D = bottoms and distillate composition in the column, respectively
z = eigenvalue optimization auxiliary variable
z_R = reactor composition
z_0 = fresh-feed composition supplied to the reactor

Greek Symbols

α = relative volatility
β_{tax}, β_{pay} = tax factor and payback period, respectively
γ = condition number
κ_i = terms in steady-state gain expressions
λ_i = eigenvalues
σ_i = singular values

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