A Nonequilibrium Stage Model of Multicomponent Separation Processes

Part IV: A Novel Approach to Packed Column Design

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Introduction

There are essentially two kinds of problems that one encounters in the literature on separation process modeling and simulation, design problems and operating or rating problems. Design calculations involve the estimation of the number of trays in a trayed column or the height of a packed column needed to achieve a desired degree of separation. Operating problems involve predicting the performance of a column of a given configuration (fixed number of stages or packed height, feed location, and so on).

In previous parts of this series we have described a nonequilibrium stage model of multicomponent separation processes (Krishnamurthy and Taylor [KT], 1985a) and used it to simulate a number of distillation and absorption processes in existing packed and trayed columns (KT, 1985b, c, 1986). In this note, we extend our approach to column simulation so that packed column design problems can be solved in an efficient manner.

Formulation of an Algorithm for Packed Column Design Calculations

When we simulate a packed column using the nonequilibrium stage model, we simply divide the column into a number of sections. The MERQ equations used to model each section of packing include (see KT, 1985a, c, for details):

M ** *M*aterial balances for each phase ($2c$ eqs.)

E ** *E*nergy balances for each phase (2 eqs.)

R ** Mass and energy transfer *R*ate models [$2(c-1)+1$ eqs.]

Q ** E*Q*uilibrium equations for the interface (c eqs.)

For a c-component system there are $5c+1$ independent equations per section (KT, 1985a).

Since the key to the proposed design method is the set of R (rate) equations, we consider these equations in more detail. Mass is transferred across the interface at rates that depend on the extent to which the two phases are not in equilibrium with each other. These rates are determined by concentration differences (Δy, Δx), by mass transfer coefficients (k, in kmol/m^2 · s or equivalent), and by the area available for interfacial transfers (A^I).

$$\mathcal{N} = k^V A^I(\Delta y) = k^L A^I(\Delta x) \tag{1}$$

(More rigorous expressions than this are employed in our simulations; Eq. 1 is used only to illustrate how the design algorithm is formulated.) For packed columns, the interfacial area per section, A^I, is calculated as follows from the product of the interfacial area density, a^I in m^2/m^3 of packing; the column cross-sectional area, a_c; and the height of the packed section, z_s

$$\mathcal{N} = k^V a^I a_c z_s(\Delta y) = k^L a^I a_c z_s(\Delta x) \tag{2}$$

The driving forces are calculated knowing the bulk and interface compositions (see KT, 1985a–c, for further discussion of this topic). The mass transfer coefficients and interfacial area densi-

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ties are characteristics of the equipment being used and its conditions of operation; these quantities depend on such things as the tray or packing type, flow rates, fluid properties, and so on. Correlations of mass transfer coefficients and interfacial area densities are available in the literature for a variety of packings; these correlations are used in our simulations.

If each section is assumed to have the same height (this is our usual assumption even though it is not really necessary), then the height of each section, z_s, is given by

$$z_s = H/N_s \tag{3}$$

where H is the total height of packing and N_s is the number of model sections. This number must be chosen in advance and is, to a very large extent, arbitrary. The number of sections into which the column is divided is chosen so that the height of each packed section calculated from Eq. 3 is appropriate. To a large extent, experience plays a role here. In some of our earlier work, we found that large packed columns could be modeled using only a few nonequilibrium sections in order to meet a particular accuracy in the numerical solution (KT, 1985c). Increasing the number of model sections beyond a certain value had little or no effect on the results of a simulation, although it did have quite an impact on the computer time requirements.

In a column simulation the height of the column is known; in a design problem, the column height is not known and therefore, even if N_s has been chosen, z_s cannot be calculated in advance. The conventional way out of this difficulty would be to estimate the height, perform a simulation calculation, examine the results, and then repeat the exercise as often as needed until we have met the design criteria. This is very time-consuming. In the method we have developed for performing design calculations, N_s is chosen in advance (precisely as we would do if we were solving an operating problem) and z_s is regarded as an additional variable, its value determined by solving a design specification equation simultaneously with the MERQ equations for all of the nonequilibrium model stages. As a result, we usually are able to solve design problems in less time than is needed to solve two equivalent operating problems.

A common absorber design problem involves the determination of the height needed to produce a product of a particular purity. In this case, the design equation takes the form

$$D \equiv v_{i1} - v_{i,\text{spec}} = 0 \tag{4}$$

where the sections are numbered from the top down. Other specifications are possible, of course.

For an absorber design problem, the total number of equations being solved is $N_s(5c + 1) + 1$. As in our earlier work, we solve all of these equations simultaneously using Newton's method (see KT, 1985a, for a discussion of its application in solving the MERQ equations of the nonequilibrium stage model). The structure of the Jacobian matrix for an absorber simulation was discussed in part I of this series (KT, 1985a). For a design problem, the Jacobian has the structure shown in Figure 1. It is interesting to note that the design equation does not depend on the design variable z_s. Thus, the lower righthand corner element of the Jacobian matrix is zero. The Jacobian is not, however, singular; the bottom row contains a single nonzero element (corresponding to the derivative of the design equation

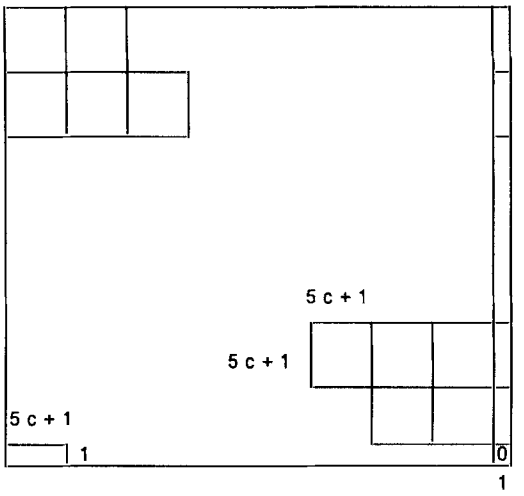

Figure 1. Structure of Jacobian matrix for an absorber design problem.
Numbers indicate dimension of submatrices, except 0, which is the value of that element.

with respect to the component flow rates appearing in the equation) and the righthand column is about 40% full, containing the derivatives of the mass (and energy) transfer rate equations with respect to z_s that appear in the calculation of the interfacial area, Eq. 2. Upon convergence, the calculated height per section is multiplied by the specified number of sections to give the total packed height.

It should be emphasized that we do not adjust the number of model sections between iterations; that is, the number of equations being solved is chosen in advance and maintained constant until the numerical problem has been solved. This means that no variables (for which we would need to generate new starting guesses) are added to or subtracted from the problem nor do we have to redefine the sparsity pattern of the Jacobian between iterations.

The same approach could be used for distillation design problems where two specification equations (for two product streams or for one product and an optimum feed location specification equation) would augment the set of MERQ equations for each section of packing. The height of a section in the lower part of the column and the height of a section in the upper part of the column would be the additional variables.

Numerical Results

To illustrate the method, we consider the determination of the height of packing needed to remove CO_2 from a sour gas feed with refrigerated methanol as the solvent. The sour gas feed consisted of from three to ten components taken from CO_2, H_2S, COS, N_2, H_2, and various hydrocarbons. An extensive experimental and theoretical investigation of this process has been described by Kelly (1981) and by Kelly et al. (1984). The problem here is to estimate the height required to absorb the amounts of CO_2 absorbed in each of the experiments of Kelly et al. A total of 16 packed columns have been designed mathematically using the approach described above. For these calculations, the packed height was divided into six sections of equal length for the three-component problems and eight sections for the eight- and ten-component problems. Physical properties and

Table 1. Results of Packed Column Design for Absorption of Acid Gases Using Methanol

Run No.	Height, Calc. by: Proposed Method m	Height, Calc. by: Kelly m	No. Iterations for Design Method	No. Iterations for One Equiv. Operating Problem
		3-Component System		
AM 24	0.7925	0.8769	13	8
AM 25	0.8122	1.0153	12	8
AM 26	1.6275	1.3850	13	8
AM 27	1.8048	*	15	9
AM 32	0.5933	0.7459	13	9
AM 33	0.5038	0.6507	12	9
AM 34	0.6434	0.7964	12	7
AM 38	0.6631	0.7324	13	7
AM 50	0.8838	0.8833	16	7
AM 55	1.1702	*	16	7
		8-Component System		
AM 30	0.4434	0.4316	10	7
AM 35	0.4743	0.4575	15	9
AM 36	0.7136	0.5000	14	7
AM 37	0.4208	0.3908	13	8
AM 52	0.4850	0.3011	18	7
		10-Component System		
AM 59	0.5194	0.4703	12	7

*No convergence, because calculated liquid to gas flow ratio was below the minimum.

transport coefficients were calculated as described elsewhere (KT, 1986).

Results of the 16 packed column design problems are given in Table 1. Packing heights computed using the nonequilibrium design method for various runs are compared with those computed by Kelly, who used the method of Feintuch and Treybal (1978). That method involves the numerical solution of a set of nonlinear differential equations and is equivalent to the repeated solution of column simulation problems with the process model equations solved using a stage-to-stage method. The reason for the sometimes quite large discrepancy between our results and those of Kelly is that the temperature profile, which is quite steep near the bottom of the column, flattens out in the upper part of the column as the CO_2 is almost completely absorbed (99% in many cases); consequently, the computed height is somewhat sensitive to the many parameters that appear in the MERQ equations. We did not use the same physical property models that Kelly used, nor did we use the same mass and heat transfer rate models. Elsewhere, we have shown that our nonequilibrium stage model is able to predict the experimentally observed temperature profiles to a quite satisfactory degree of accuracy (KT, 1986); thus, we believe our choice of property and transport models to be reasonable. It may also be pertinent to note that Kelly was not able to obtain a solution for runs AM 27 and AM 55 due to the liquid to gas flow ratio being computed to be below the minimum (even though the column certainly operated at those conditions). No difficulties were encountered with the present method.

Table 1 also summarizes the main results of this investigation, the number of iterations needed to solve an equivalent operating problem. In almost all cases investigated, the computational effort required for the design problem is less than that required by two equivalent operating problems. This is much less than the number of different operating problems that normally have to be solved to meet design criteria.

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Notation

a' = interfacial area density, m^2/m^3 of packing
a_c = column cross-sectional area, m^2
c = number of components
D = design equation
H = total height of packing (m)
k = mass transfer coefficient (kmol · m^{-2} · s^{-1})
K = equilibrium ratio
$\mathcal{N}$ = rate of transfer of species across interface, kmol · s^{-1}
N_s = number of model stages
v = vapor flow rate (kmol · s^{-1})
x = liquid phase composition
y = vapor phase composition
z_s = height of a section of packing, m

Superscripts and subscripts

I = interface
L = liquid
V = vapor
i = component index

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