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The steady state model of a reactive distillation column for ethylene glycol synthesis is presented here, taken from CIRIC & MIAO [1]. The second reaction is neglected as in subsection *7.3. Multiple reactions* of that paper. The index for the reactions is omitted since only one reaction remains.

Parameters

C	number of components	$C = 3$
N	number of stages	$N = 10$
f_{ij}	feed flow rates	$i = 1 \dots C, \quad j = 1 \dots N$
ν_i	stoichiometric coefficients	$i = 1 \dots C$
λ	homotopy parameter	
W_j	reaction volume	$j = 1 \dots N$
H_{vap}	heat of vaporization	
H_r	heat of reaction	
β	reboiler boil-up ratio	

Variables

x_{ij}	liquid phase composition	$i = 1 \dots C, \quad j = 1 \dots N+1$
y_{ij}	vapor phase composition	$i = 1 \dots C, \quad j = 0 \dots N$
l_{ij}	liquid phase component molar flowrate	$i = 1 \dots C, \quad j = 1 \dots N+1$
v_{ij}	vapor phase component molar flowrate	$i = 1 \dots C, \quad j = 0 \dots N$
L_j	liquid phase molar flowrate	$j = 1 \dots N+1$
V_j	vapor phase molar flowrate	$j = 0 \dots N$
T_j	temperature at stage j	$j = 1 \dots N$
ξ_j	extent of reaction at stage j	$j = 1 \dots N$

Equations

Molar flowrates to simplify the notation

$$l_{ij} := x_{ij} L_j \quad \text{for } i = 1 \dots C, \quad j = 1 \dots N+1 \tag{1}$$

$$v_{ij} := y_{ij} V_j \quad \text{for } i = 1 \dots C, \quad j = 0 \dots N \tag{2}$$

Condenser

$$L_{N+1} = V_N \tag{3}$$

$$x_{i,N+1} = y_{i,N} \quad \text{for } i = 1 \dots C \tag{4}$$

Reboiler

$$V_0 = \beta L_1 \quad (\beta \text{ from specification}) \tag{5}$$

$$y_{i,0} = x_{i,1} \quad \text{for } i = 1 \dots C \tag{6}$$

Phase equilibrium

$$y_{ij} = K_i(T_j) x_{ij} \quad \text{for } i = 1 \dots C, \quad j = 1 \dots N \tag{7}$$

Extent of reaction

$$\xi_j = \lambda W_j f(x_{1j}, \dots, x_{C,j}, T_j) \quad \text{for } j = 1 \dots N \tag{8}$$

Material balances

$$f_{ij} + v_{i,j-1} + l_{i,j+1} + \nu_i \xi_j = v_{ij} + l_{ij} \quad \text{for } i = 1 \dots C, \quad j = 1 \dots N \tag{9}$$

Heat balances

$$H_{\text{vap}}(V_{j-1} - V_j) = H_r \xi_j \quad \text{for } j = 1 \dots N \tag{10}$$

Summation equations

$$\sum_{i=1}^{C} x_{ij} = 1 \quad \text{for } j = 1 \dots N \tag{11}$$

$$\sum_{i=1}^{C} y_{ij} = 1 \quad \text{for } j = 1 \dots N \tag{12}$$

Elimination order. Let introduce the following notation

$$\xi_{\text{tot}} := \sum_j \xi_j \quad \text{(overall extent of reaction).} \tag{13}$$

Once a value for ξ_{tot} is assumed, everything else can be computed by solving univariate equations. This makes the problem essentially 1-dimensional. However, solving it as a 1-dimensional zero-finding problem does not work. The equations show extreme sensitivity to the value of ξ_{tot}.

Let

$$b_i := l_{i,1} - v_{i,0} \quad \text{for } i = 1 \dots C \quad \text{(bulk component flowrate).} \tag{14}$$

The sum of all equations (9) over $j = 1 \dots N$, also taking into account (1)–(4) and (11), (12), is

$$\sum_j f_{ij} = l_{i,1} - v_{i,0} - \nu_i \sum_j \xi_j \quad \text{for } i = 1 \dots C. \tag{15}$$

Once a value is assumed for ξ_{tot} the elimination is started as follows. Solve (15) for the b_i:

$$b_i = \sum_{j=1}^{N} f_{ij} + \nu_i \xi_{\text{tot}} \quad \text{for } i = 1 \ldots C. \tag{16}$$

From (1), (2) and (5), (6) we have

$$l_{i,1} = \frac{1}{1-\beta} b_i \quad \text{for } i = 1 \ldots C,$$

$$v_{i,0} = \frac{\beta}{1-\beta} b_i \quad \text{for } i = 1 \ldots C.$$

At this point, everything is known to start the stage-by-stage propagation, working from $j = 1$ to $j = N$.

Find $l_{i,j+1}$ and $v_{i,j}$ given l_{ij} and $v_{i,j-1}$ (going from stage j to $j+1$). First,

$$x_{ij} = \frac{l_{ij}}{\sum_i l_{ij}}. \tag{17}$$

Solve

$$\sum_i K_i(T_j) x_{ij} = 1 \tag{18}$$

for T_j. Then perfom the elmination in the order given below.

$$y_{ij} = K_i(T_j) x_{ij} \quad \text{for } i = 1 \ldots C \tag{19}$$

$$\xi_j = W_j f(x_{1j}, \ldots, x_{C,j}, T_j) \tag{20}$$

$$V_{j-1} = \sum_i v_{i,j-1} \tag{21}$$

$$V_j = -\frac{H_r \xi_j}{H_{\text{vap}}} + V_{j-1} \tag{22}$$

$$v_{ij} = y_{ij} V_j \quad \text{for } i = 1 \ldots C \tag{23}$$

$$l_{i,j+1} = v_{ij} + l_{ij} - \nu_i \xi_j - (f_{ij} + v_{i,j-1}) \quad \text{for } i = 1 \ldots C \tag{24}$$

Finally,

$$\sum_i l_{i,N+1} = \sum_i v_{i,N}. \tag{25}$$

This is the final equation, depending only on ξ_{tot}.

References

[1] Amy R. Ciric and Peizhi Miao. Steady state multiplicities in an ethylene glycol reactive distillation column. *Ind. Eng. Chem. Res.*, 33:2738–2748, 1994.