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Reaction Distillation with Ion Exchangers

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Abstract

This paper studies batch distillation with reaction esterification of acetic acid and ethanol. The experimental investigation was carried out at atmospheric pressure in a column packed with ion exchanger Amberlite-120. The mathematical model was established by introducing reaction functions in material and enthalpy balance equations. The results obtained for the startup and product periods show advantages for reaction distillation with ion-exchange catalysis. A clean product is obtained, and there is no problem of wastewater or corrosion.

INTRODUCTION

Compared to the processes in regular distillation columns, the processes in reaction columns are extremely complex. The combination of a reversible reaction in the liquid phase and distillation is a widely used technique to enhançe the conversion of reactants to levels above those of equilibrium conversion. The choice of optimum equipment for such a combined process is influenced by the reaction rate and by the required separation efficiency. The combination of a reversible liquid-phase reaction with distillation in a reaction column often leads to increased conversion but also has disadvantages which are particulary manifest when the reaction is catalyzed by a mineral acid. In such a case the product must be separated from the acid by vaporization, and product losses do occur (*1*, *2*). An alternative to homogeneous catalysis with mineral acid is provided by heterogeneous catalysis (*3–7*).

The effects resulting from the superposition number of reaction and distillation were studied for a number of examples (*8–21*).

In this paper the effects of separation, esterification rate, and ion-exchange reactions are investigated. The mathematical models were established by introducing reaction functions in material and enthalpy balance equations for startup and product periods. An algorithm and program were developed to solve the equations by using the two-point implicit method and the multi-θ–η method with the Newton–Raphson technique of convergence. The results of the present investigation show that the reversible esterification reaction of acetic acid and ethanol in the ion-exchangers packed bed in a distillation column accelerates, yields a clean product, and has no problem of wastewater and corrosion.

THE SEPARATION PROCESS

Mass transfer with chemical reaction takes place between two phases in an ion-exchange bed. The physical and chemical equilibrium are very complex in distillation processes with a reaction esterification. The combination of a slow esterification reaction as a reversible liquid-phase reaction with distillation in a reaction column leads to increased conversion.

Vapor–Liquid Equilibrium

When the vapor and liquid phases are in physical equilibrium at a given temperature and pressure, the fugacity of component *i* in the vapor phase is equal to the fugacity of component *i* in the liquid phase:

$$f_{ji}^{V} = f_{ji}^{L} \qquad (i = 1, 2, 3, \ldots, n;\ j = 1, 2, \ldots, N) \tag{1}$$

or

$$\begin{aligned} f_{ji}^{oV}\phi_{ii}y_{ji} &= f_{j}^{oL}\gamma_{ji}x_{ji} \\ y_{ji} &= \gamma_{ji}K_{ji}x_{ji} \end{aligned} \tag{2}$$

where K_i is the ideal solution K value, $K_{ji} = f_{ji}^{oL}/f_{ji}^{oV}$ and $\phi_{ij} = 1$. Since $y_i = v_i/V$ and $x_i = l_i/L$, Eq. (2) may be restated in terms of the flow rates;

$$l_i = A_i' v_i \tag{3}$$

where the absorption factors A_i' is

$$A_i' = (L_j/V_j)\gamma_{ji}K_{ij}$$

Chemical Reaction Function

Let a reaction occur in the liquid phase

$$a\text{A} + b\text{B} \rightleftarrows c\text{C} + d\text{D} \tag{4}$$

This reaction can be restated in the following equivalent form:

$$\nu_A A + \nu_B B + \nu_C C + \nu_D D = 0 \tag{5}$$

where $\nu_A = -1$, $\nu_B = -b/a$, $\nu_C = c/a$, and $\nu_D = d/a$. Assuming that the contents are perfectly mixed, the rate of Reaction (4) is given by

$$r_{jA} = k_j c_{jA} c_{jB} - k_j' c_{jC} c_{jD} \tag{6}$$

The concentrations may be expressed in terms of the liquid flow rates as follows:

$$R_j = \frac{U_j^L (\rho_j^L)^2}{L_j^2} (k_j l_{jA} l_{jB} - k_j' k_{jC} l_{jD}) - \eta_j \tag{7}$$

where

$$\eta_j = r_{jA} U_j^L \tag{8}$$

and ρ_j^L is the molar density of the liquid phase.

The chemical equilibrium for the liquid phase is expressed by the chemical equilibrium constant

$$K_{Rj}^L = \frac{(f_{jC}^L)^{\nu_C} (f_{jD}^L)^{\nu_D}}{(f_{jA}^L)^{-\nu_A} (f_{jB}^L)^{-\nu_B}} \tag{9}$$

where for the reaction

$$\underset{(A)}{CH_3COOH} + \underset{(B)}{C_2H_5OH} \rightleftarrows \underset{(C)}{CH_3COOC_2H_5} + \underset{(D)}{H_2O} \tag{10}$$

Using

$$f_{ji}^L = \frac{\gamma_{ji} f_{ji}^{oL} l_{ji}}{L_j} \tag{11}$$

and the definition of the ideal K value,

$$K = f_{ji}^L / f_{ji}^V \tag{12}$$

the following expression is obtained:

$$R_j = \frac{K_j^L K_{Kj} K_{fj}^V}{K_{Rj}^L L_j} - \left(\frac{l_{jC} l_{jD}}{l_{jA} l_{jB}}\right) - 1 \tag{13}$$

where

$$K_j^L = \frac{\gamma_{jC}\gamma_{jD}}{\gamma_{jA}\gamma_{jB}}, \qquad K_{Kj} = \frac{K_{jC}K_{jD}}{K_{jA}K_{jB}}, \qquad K_{fj}^V = \frac{f_{jC}^V f_{jD}^V}{f_{jA}^V f_{jB}^V}$$

Kinetics of the Ion-Exchange Reactions

Catalysis of reactions of liquid and solutes by ion exchangers can usually be explained in terms of the catalytic activity of the counterions and is analogous to homogeneous phase catalysis by dissolved electrolytes. The catalytic activity of the ion exchanger here is directly related to the ion-exchange properties of the catalyst. Reactions can be characterized by equations of the following form:

$$\mathrm{A^+resin} + \mathrm{B^+solution} \underset{k_b}{\overset{k_f}{\rightleftarrows}} \mathrm{A^+solution} + \mathrm{B^+resin} \tag{14}$$

and the rate by

$$d[\mathrm{A}_5^+ 1/dt = k_f[\mathrm{A}_r^+][\mathrm{B}_s^+] - k_b[\mathrm{A}_s^+][\mathrm{B}_r^+] \tag{15}$$

where r and s stand for resin and solution, the brackets represent concentrations, and k_f and k_b are the rate constants for the forward and reverse reactions, respectively.

In this consideration, diffusion controlled kinetics was neglected (*22*, *23*).

THE PROCESS MODEL

The mathematical model for a catalyzed distillation reaction is based on the material and enthalpy balances, physical equilibrium relationships, and the chemical equilibrium expressions.

The physical equilibrium equation is given by

$$y_{ji} - \gamma_{ji} K_{ji} x_{ji} = 0 \tag{16}$$

and the absorption factor by

$$A_i^j = (L_j/V_j)\gamma_{ji} K_{ji} \tag{17}$$

The vapor–liquid equilibrium data for an acetic acid–ethanol–ethyl acetate–water system are taken from Suzuki et al. (*24*) and Hirata et al. (*25*) (Appendix 1).

The superposition of the reaction esterification rate and the rate of ion exchange for macroscopic consideration can be expressed by

$$r_{j\mathrm{A}}^{(\mathrm{cat})} = k_j^{(\mathrm{cat})} c_{j\mathrm{A}} c_{j\mathrm{B}} - k_j'^{(\mathrm{cat})} c_{j\mathrm{C}} c_{j\mathrm{D}} \tag{18}$$

assuming that in the radial direction

$$k_j^{(\mathrm{cat})} = \int_0^1 f(r) k_j^{(\mathrm{cat})} r dr$$

and a mole of A reacting in unit time is given by

$$\eta_j = r_{j\mathrm{A}}^{(\mathrm{cat})} U_j^L$$

that is,

$$R_j = \frac{U_j^L (\rho_j^L)^2}{L_j^2} (k_j^{(\mathrm{cat})} l_{j\mathrm{A}} l_{j\mathrm{B}} - k_j'^{(\mathrm{cat})} l_{j\mathrm{C}} l_{j\mathrm{D}}) - \eta_j \tag{19}$$

where

$$c_{ji} = \frac{l_{ij}}{L_j/\rho_j^L}$$

The values of the reaction rate constants k and k' were taken from the paper by Arnikar et al. (*26*) for uncatalyzed esterification. For the catalyzed esterification reaction with Amberlite-120, these constants were experimentally determined in References *5* and *6* (Appendix 2).

For the startup period (total reflux), the component material balance is defined by

$$v_{j+1,i} + l_{j-1,i} - v_{ji} - l_{ji} + \nu_i \eta_j = dU_{ji}/dt \tag{20}$$

When the integral difference equations are converted to a set of algebraic equations using the two-point implicit method (*27*), the component material balances may be stated in the following matrix form:

$$\overline{A}_i \overline{v}_i = \overline{F}_i - \overline{\nu}_i \overline{\eta} \tag{21}$$

The θ method of the convergence for the startup period is defined as

$$\frac{U_{ji}}{U_{l,i}} = \theta_j \left(\frac{U_{ji}}{U_{l,i}} \right)_{ca} \qquad (j = 2, 3, \ldots, N) \tag{22}$$

In order to avoid numerical difficulties in the application of the θ method, a new variable, p_i, should be introduced, as demonstrated for columns at steady-state operation:

$$p_i = \frac{U_{FO} X_{Fi} + \sum_{j=1}^{N} \nu_i \eta_j \Delta t + \xi(t_n)}{(U_{ji})_{ca} + \theta \sum_{j=2}^{N} (U_{ji})_{ca}} \tag{23}$$

Then the mole fractions are readily computed as follows:

$$x_{ji} = \frac{(U_{ji})_{ca} p_i}{\sum_{i=1}^{n} (U_{ji})_{ca} p_i} \tag{24}$$

and

$$y_{ji} = \frac{(U_{ji})_{ca} p_i K_{ji} \gamma_{ji}}{\sum_{i=1}^{n} (U_{ji})_{ca} p_i K_{ji} \gamma_{ji}} \tag{25}$$

The total enthalpy balance is given by

$$Q_r - Q_{CO} + \sum_{j=1}^{N} \eta_j \sum_{j=1}^{n} \nu_i \hat{h}_{ij} = \frac{d\left(\sum_{j=1}^{N} \sum_{i=1}^{n} \hat{h}_{ij} U_{ij} \right)}{dt} \tag{26}$$

For the product period ($B = 0$, $D > 0$), the holdup U_N decreases as the product period progresses. When the component material balances are written for each stage and the resulting integral-difference equations are converted to algebraic form by using the implicit method, the system of equations may be represented by matrix Eq. (21) by replacing l_{1i} by $v_{1i} = d_i$.

The θ method of convergence for the product period is defined as follows:

$$\frac{U_{Ni}}{d_i} = \theta_0 \left(\frac{U_{Ni}}{d_i}\right)_{ca}, \qquad \text{for } j = N$$
$$\frac{U_{ji}}{d_i} = \theta_1 \left(\frac{U_{ji}}{d_i}\right)_{ca}, \qquad \text{for } j = 1, \ldots, N-1 \tag{27}$$

By using the two-point implicit method, the following is obtained:

$$d_i = \frac{\left(-d_i^\circ + \sum_{i=1}^{N} \nu_i \eta_i^\circ\right) + \sum_{i=1}^{N} \nu_i \eta_j + \frac{1}{\phi \Delta t} \sum_{j=1}^{N} U_{ji}^\circ}{1 + \frac{1}{\phi \Delta t}\left[\theta_0 \left(\frac{U_{Ni}}{d_i}\right)_{ca} + \theta_1 \sum_{j=1}^{N-1} \left(\frac{U_{ji}}{d_i}\right)_{ca}\right]} \tag{28}$$

In order to avoid numerical difficulties in the application of the θ-method, a new variable p_i should be introduced:

$$p_i = \frac{\sigma\left(-d_i^\circ + \sum_{i=1}^{N} \nu_i \eta_i^\circ\right) + \sum_{i=1}^{N} \nu_i \eta_j + \frac{1}{\phi \Delta t} \sum_{j=1}^{N} U_{ji}^\circ}{(d_i)_{ca} + \frac{1}{\phi \Delta t}\left[\theta_0 (U_{Ni})_{ca} + \theta_1 \sum_{j=1}^{N-1} (U_{ji})_{ca}\right]} \tag{29}$$

The mole fractions are computed by using Eqs. (24) and (25).

Based on the temperature and L/V profiles, the material balances, the physical equilibrium relationships, and the chemical equilibrium expressions are solved for the moles of each component which react per unit time in the column by using the Newton–Raphson technique (*27*, *28*). The calculations were carried out for a large number of time periods.

VLE data for the acetic acid–ethanol–ethyl acetate–water system were taken from References *24* and *25* (Appendix 1). Enthalpy data were taken from References *29* and *30* (Appendix 3).

According to the established mathematical model, algorithm and computer programs were used for the analysis and simulation of the esterification rate and separation efficiency. The program package was written in BASIC and tested on an IBM PC/XT/AT compatible computer.

EXPERIMENTAL MEASUREMENTS

The experimental investigations were performed in a ordinary glass "Normag" column with a packing height of 1000 mm and a diameter of

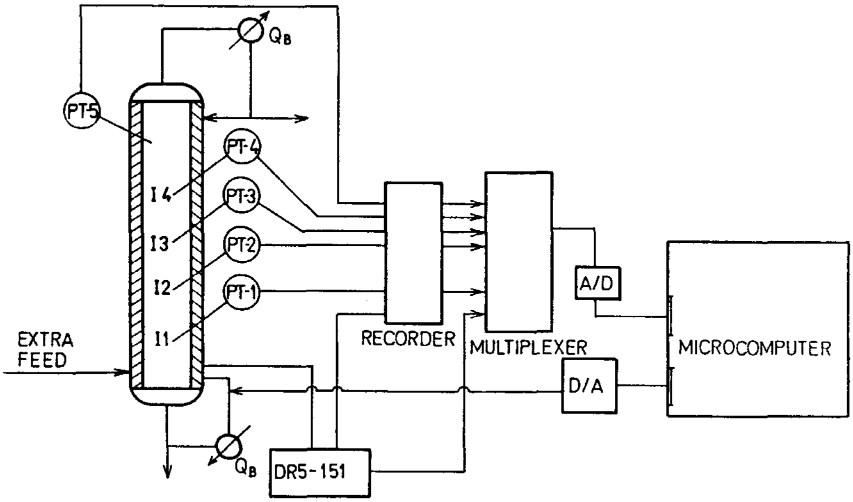

FIG. 1. Sketch of the apparatus.

33 mm. Catonic ion exchanger Amberlite-120 has an average diameter of 0.8 mm. The bed void fraction was 0.6, and the specific surface of packing was 7.056 mm^2/mm^3.

The process set-up is shown in Fig. 1. The batch distillation unit is controlled by the acquisition block. The acquisition unit performs direct measurements and controls the temperatures with sensors Pt-100 and the pressure drop with DRP-151. An Iskra-Delta microcomputer was used.

The experiments were carried out by a batchwise distillation operation and were semicontinuous in adiabatic conditions. The charge consisted of 50 mol% acetic and 50 mol% ethanol. The compositions of the distillate and the bottom product were determined by gas chromatography.

The distillation was performed at different flow rates through the column. The optimal flow rate through the column was investigated. The hydrodynamic characteristics with a cationic ion exchanger were determined previously (*6*).

RESULTS AND DISCUSSION

The results obtained are presented in Figs. 2–5. The composition of the distillate for different flow rates is shown in Fig. 2. The optimal flow rate for the column investigated was W_{op} = 1.8 m/s.

The temperature profile through the column 1 hour after the startup process period is shown in Fig. 3. Comparison of the experimental and calculated temperatures shows good agreement.

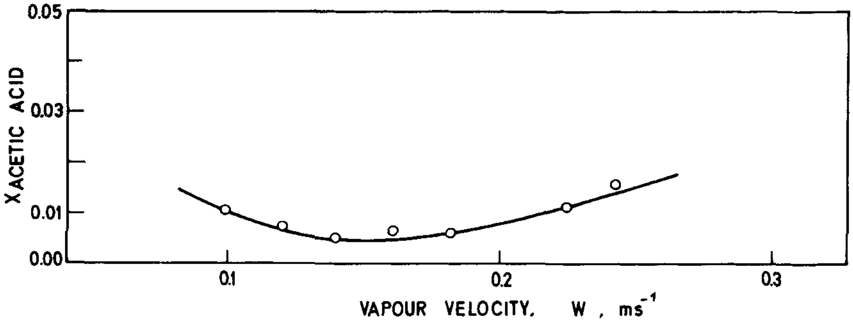

FIG. 2. The distillate composition vs flow rates.

The distillate composition vs time for the startup period is shown in Fig. 4. A constant distillate composition is achieved after 1 hour. The distillate composition vs time for the product period is shown in Fig. 5. A constant distillate composition is achieved in the product period because the combination of reversibile reaction esterification with the multistage distillation operation leads to increased conversion. Comparison of the experimental and calculated compositions shows good agreement.

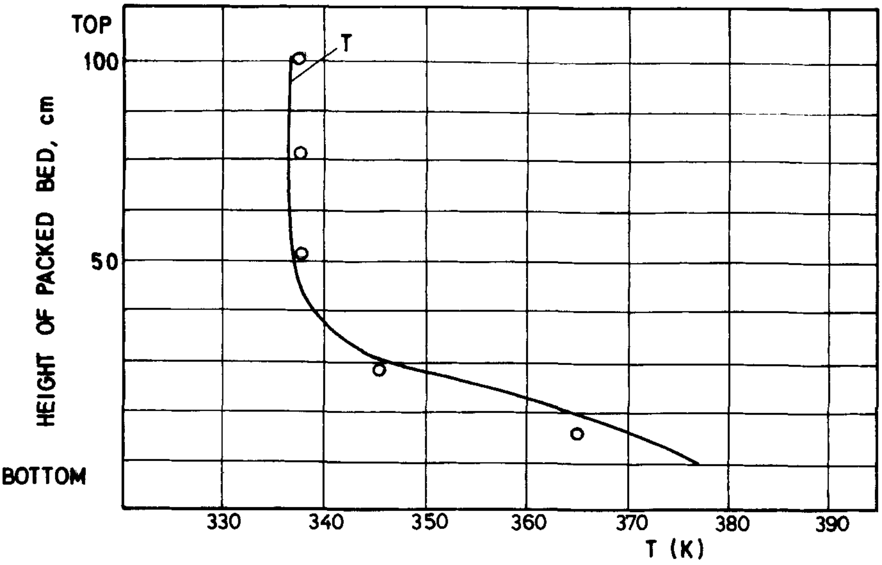

FIG. 3. The temperature profiles through the column 1 hour after the startup process: (o) experimental, (—) calculated.

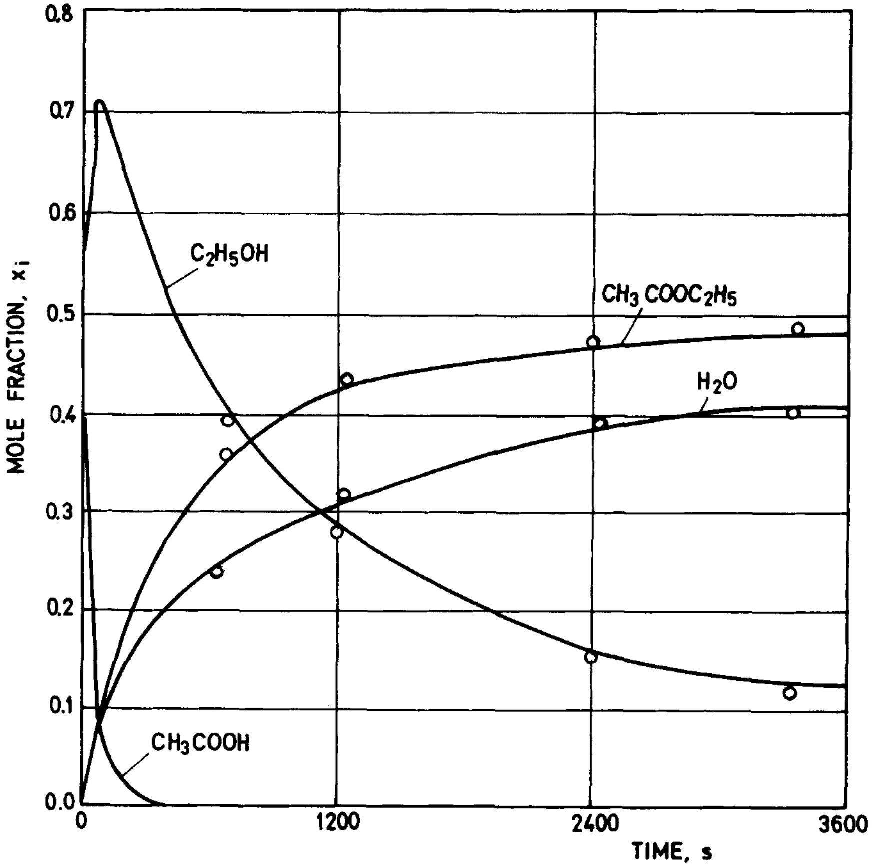

FIG. 4. The distillate composition vs time for the startup period: (o) experimental, (——) calculated.

CONCLUSION

The results obtained show that heterogeneous catalysis with the catonic ion exchanger Amberlite-120 accelerates the esterification reaction in a distillation column. Analyses of the results of the startup and product periods show the advantages of catalyzed reaction distillation with ion exchangers: a clean product of constant quality is obtained, there are no wastewater or corrosion problems, and there is the possibility of multiple use.

We examined the reaction separation method by using the heterogeneous catalyst Amberlite-120. The results show that the reversibile esterification

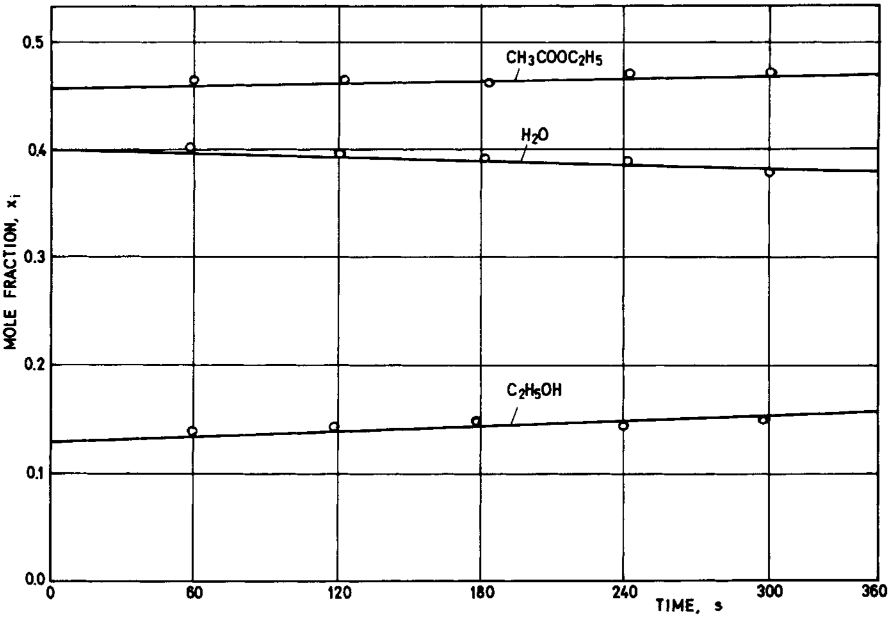

FIG. 5. The distillate composition vs time for the product period: (○) experimental, (——) calculated.

reaction of acetic acid and ethanol in the ion-exchanger packed bed of the distillation column is accelerated, and the product must not be subsequently separated from the impurities. We note that the pressure drop in the ion-exchanger packed bed is much higher than in the classical packed bed (Rashig rings).

APPENDIX 1. VAPOR–LIQUID EQUILIBRIUM DATA

Activity coefficients were determined by the following equation:

$$\log_{10}\gamma_1 = A_1x_2^2 + A_2x_3^2 + A_3x_4^2 + A_4x_2x_3 + A_5x_2x_4 + A_6x_3x_4 + A_7x_1x_2^2 + A_8x_1x_3^2 + A_9x_1x_4^2 + A_{10}x_1x_2x_3 + A_{11}x_2x_3x_4 + A_{12}x_3x_4x_1 + A_{13}x_4x_1x_2 + A_{14}x_2x_3^2 + A_{15}x_2x_4^2 + A_{16}x_3x_4^2 \qquad (A1.1)$$

The remaining activity is obtained from the subscripts on the x's as follows: 1 → 2 → 3 → 4 → 1. $A_1 \rightarrow A_{16}$ are empiric constants. See Table A1.1.

TABLE A1.1
Coefficients in Eq. (A1.1)

A_i	CH_3COOH (1)	C_2H_5OH (2)	H_2O (3)	$CH_3COOC_2H_5$ (4)
1	−0.554296	0.581778	0.688636	−0.0601361
2	−0.324357	0.209245	0.0243031	0.229575
3	−0.103685	−0.257329	0.375534	1.86575
4	−0.705455	−0.562636	1.27548	0.355191
5	−2.01335	−0.314853	1.77863	0.468416
6	−2.25362	0.451732	0.696279	1.51110
7	0.837926	−0.115411	0.936722	−0.0599682
8	0.523760	0.069531	0.449357	0.0673994
9	0.434061	0.0740529	0.717790	−3.15997
10	−0.534056	0.187010	1.44979	0.941858
11	−3.25231	−0.369985	−2.11099	−1.92225
12	5.90329	−0.082339	0.746905	−0.755731
13	3.35400	−0.409472	1.12914	1.03791
14	0.197296	1.09247	0.120436	0.365254
15	−0.452660	0.192416	−1.64268	−1.36587
16	0.014715	−0.172565	0.330018	−2.13818

Vapor–liquid equilibrium data are given in Table A1.2.

APPENDIX 2. CHEMICAL REACTION DATA

$$\underset{(A)}{CH_3COOH} + \underset{(B)}{C_2H_5OH} \underset{k'}{\overset{k}{\rightleftarrows}} \underset{(C)}{CH_3COOC_2H_5} + \underset{(D)}{H_2O}$$

$$r_{jA} = k_{jA}c_Ac_B - k'_{jA}c_Cc_D \ \mathrm{mol{\cdot}L^{-1}{\cdot}min^{-1}}$$

TABLE A1.2
Vapor–Liquid Equilibrium Data

Component	VLE ratio	
1	$K = 2.25 \times 10^{-2} \cdot t - 1.666$	$t > 74.45$
	$K = 0.001$	< 74.45
2	$\log K = -2.3 \times 10^3/T + 6.58825$	
3	$\log K = -2.3 \times 10^3/T + 6.48351$	
4	$\log K = -2.3 \times 10^3/T + 6.74151$	

where

$$k_{jA} = 29.000 \exp\,(-7150/T)\ \mathrm{L{\cdot}mol^{-1}{\cdot}min^{-1}} \tag{A2.1}$$

$$k'_{jA} = 7.380 \exp\,(-7150/T)\ \mathrm{L{\cdot}mol^{-1}{\cdot}min^{-1}} \tag{A2.2}$$

for uncatalyzed reaction esterification (*26*).

The constants for catalyzed reaction esterification with ion exchanger Amberlite-120 (*6*) are

$$k_{jA}^{(cat)} = 58.7 \times 10^{-3} \exp\,(-17.46/T)\ \mathrm{L{\cdot}mol^{-1}{\cdot}min^{-1}} \tag{A2.3}$$

$$k_{jA}^{\prime(cat)} = 22.1 \times 10^{-3} \exp\,(-16.53/T)\ \mathrm{L{\cdot}mol^{-1}{\cdot}min^{-1}} \tag{A2.4}$$

APPENDIX 3. VAPOR AND LIQUID ENTHALPIES

The vapor and liquid enthalpies were calculated by using the following values of the virtual values of the partial molar enthalpies.

$$\hat{H}_i = H_i^\circ + \Omega \tag{A3.1}$$

$$\hat{h}_i = \hat{H}_i + \lambda_i(\mathrm{T}) \tag{A3.2}$$

where

$$\Omega = -RGT^2 \left(\frac{\partial \log_e f}{\partial T}\right)_{P,n}$$

The following expression, based on the BWR equation of state, was used for computing:

$$\Omega = (B_0RGT - 2A_0 - 4C_0/T^2) + (2bRG - 3a)\rho^2/2 + \frac{6a\alpha\rho^5}{5} + \frac{c\rho^2}{T^2}\,3\left[\frac{1 - \exp\,(-\Gamma\rho^2)}{2} - \frac{\exp\,(-\Gamma\rho^2)}{2} + \Gamma\rho^2 \exp\,(-\Gamma\rho^2)\right] \tag{A3.3}$$

where B_0, A_0, C_0, a, b, c, α, and Γ are constants in the BWR equation, and H_i° is the vapor enthalpy of the pure component. See Tables A3.1 and A3.2.

TABLE A3.1
Constants in the BWR Equation

	CH_3COOH (1)	C_2H_5OH (2)	H_2O (3)	$CH_3COOC_2H_5$ (4)
B_0	1.04651	0.81653	0.29786	1.39142
A_0	38041.33	26001.91	1.178×10^4	4.452×10^4
C_0	3.83×10^{10}	1.97×10^{10}	1.40×10^{10}	3.47×10^{10}
b	6.96508	4.31489	0.5643	12.31281
a	94930.17	51071.14	8368.41	147709.5
c	1.593×10^{11}	6.46×10^{10}	1.66×10^{10}	1.92×10^{11}
α	6.2865×10^5	1.6491×10^5	1.2778×10^3	2.2991×10^6
Γ	11.2486	6.9685	0.91127	19.885

Latent Heat of Vaporization

Latent heats of vaporization (25) are given by

$$\lambda_{i2} = \lambda_{i1}\left[\frac{1 - T_{r2}}{1 - T_{r1}}\right]^{0.38}, \quad T_r = T/T_c \qquad \text{(A3.8)}$$

See Table A3.3.

SYMBOLS

A'	absorption factor
A	acetic acid
A	tridiagonal matrix
A^+	cation in ion-exchange reaction
B	ethanol

TABLE A3.2
Enthalpy Data for the Perfect Gas State

Component	$H_i^\circ = \Delta H_{298}^\circ + T_{298}C_p^\circ\, dT$ cal/mol (or × 4.186 J/mol)	
1	$H_1^\circ = -106607.89 + 1.156T + 3.0435 \times 10^{-2}T^2 - 1.3956 \times 10^{-5}T^3 + 2.955 \times 10^{-9}T^4$	(A3.4)
2	$H_2^\circ = -58855.738 + 2.153T + 2.5565 \times 10^{-2}T^2 - 6.68 \times 10^{-6}T^3 + 8.2 \times 10^{-11}T^4$	(A3.5)
3	$H_3^\circ = 60135.845 + 7.701T + 2.2975 \times 10^{-4}T^2 - 8.4 \times 10^{-7}T^3 + 2.15 \times 10^{-10}T^4$	(A3.6)
4	$H_4^\circ = -110238.9 + 1.1728T + 4.8625T^2 - 1.665 \times 10^{-5}T^3 + 1.729 \times 10^{-9}T^4$	(A3.7)

TABLE A3.3
Latent Heats of Vaporization and Other Properties

Component	Latent heats of vaporization at boiling point λ_i cal·mol (or × 4.186 J/mol)	$T_{B.P}$ (K)	Critical temperature (K)	Molar density ρ (mol/cm^3)
1	5660	391.1	594.4	0.017470
2	9260	351.5	516.2	0.017129
3	9717	373.2	647.3	0.055490
4	7700	350.3	523.2	0.010220

B^+	cation in ion-exchange reaction
C	ester
c	concentration (mol/L)
D	water
D'	distillate
f	fugacity
F	vector of terms of the component material balance of the two-point implicity method
$\hat{h}$, $\hat{H}$	virtual value of the partial molar enthalpy in the liquid and vapor phases, respectively (J/mol)
K	ideal solution K value, $K_{ji} = f_{ji}^{oL}/f_{ij}^{oV}$
k	rate constant of second-order forward reaction (L·mol^{-1}·min^{-1})
k'	rate constant of second-order reverse reaction (L·mol^{-1}·min^{-1})
k_f, k_b	ion exchange rate constant
l	molar flow rate in the liquid phase (mol/min)
L	total molar flow rate in the liquid phase (mol/min)
N	total column height
n	total number of component
p_{io}	saturated vapor pressure
P	total pressure
Q	heat (J)
R	reaction function
T, t	temperature, K and °C, respectively
t_n	time
r_{jA}	rate of reaction of the base component A; moles of A reacted per unit volume in the conditions of unit j (mol·L^{-1}·min^{-1})

RG	gas constant
v	molar flow rate in the vapor phase (mol/min)
V	total molar flow rate (mol/min)
U	volumetric holdup (mol)
x	liquid-phase mole fraction
y	vapor-phase mole fraction
z	column height
Z	parameter (between -3 and 6)

Greek Letters

γ	activity coefficient
Δt	interval of time
η	number of moles of the base component A reacted per unit time
ν	mole ratio defined by Eq. (5)
$\xi\ (tn)$	mole of base component A reacted in previous intervals of time
ϕ	factor ($\phi = 0.6$) for the two-point implicit method
θ, θ_0, θ_1	multiplier defined by Eqs. (22) and (27)
ρ	molar density
σ	$(1 - \phi)/\phi$
Ω	a function of temperature, pressure, and composition; Eq. (A3.3)
λ	latent heat of vaporization

Subscripts

i	component number
j	unit of packed bed height
A, B, C, D	components
CO	condenser
ca	calculated values
co	corrected values
r	reboiler
FO	feed charge
s	solution
r	resin

Superscripts

V	vapor phase
L	liquid phase

o	state of variables in interval *tn* + Δt
–	matrix form
+	cation
cat	catalyzed

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