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COMPARISON OF THE EFFICIENCY OF MASS EXCHANGE IN THE COMPLEX MODEL FOR HIGHLY VOLATILE AND NONVOLATILE COMPONENTS

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The efficiencies of mass exchange in the complex model have been compared for two variants of representation of the running equation of the equilibrium line: $y = mx$ *and* $y = ax + b$*. Based on the processing of experimental data on separation of the benzene–toluene mixture in cross motion of the flows, it has been shown that the first equation is adequate only for small variations in the concentrations at the step of mass-exchange while the second equation has a more universal character.*

General propositions of the complex mass-exchange model as applied to rectification processes and the basic calculation dependences have been given in [1–3]. This model differs from the existing models of Murphree and Hausen [4–7] in the conditions of the relationship between the ideal and real plates when the compositions of the flows on these plates are equalized at a certain distance h for the vapor and h_1 for the liquid from the site of their injection. It has been proposed [8] that the change in the distances h and h_1 be taken the same and be found as a function of the coefficient of phase equilibrium

$$h = h_1 = \frac{1}{m+1}, \tag{1}$$

which imparts a dynamic character to the model and transforms the calculation formulas depending on the coefficient of phase equilibrium changing with the column height.

In the present work, it is proved that the efficiency of mass exchange has the same values in the complex model in calculating from the parameters of highly volatile and nonvolatile components.

The running equation of the equilibrium line can be represented by the expressions

$$y = mx, \tag{2}$$

$$y = ax + b, \tag{3}$$

The running slope of the equilibrium line is equal to the coefficient of phase equilibrium; however the first of the above formulas is simpler in employment and its use can result in significant errors, especially in the case of a large difference of the concentrations of the components arriving at the contact step and coming out of it.

Let us consider the nth plate in a total-reflux column in which the molar vapor and liquid flows are the same ($L = V$). The working line of such a column on the y–x diagram is represented by the diagonal line ON (Fig. 1). We draw the straight lines OK and OM from the origin of coordinates in such a manner that they intersect the equilibrium curves OAN and OBN at points A and B characterized by the contact of, respectively, the highly volatile and nonvolatile components in the liquid x_{n-1} and x'_{n-1} ($x_{n-1} = 1 - x'_{n-1}$). The straight lines OK and OM are constructed from the running equations of equilibrium for the nth plate. In the case of their use, the difference $x_n - \dfrac{y_{n-1}}{m}$ employed in the calculation dependences and presented by segment CP in Fig. 1 turns out to be somewhat understated (by Δ) for the

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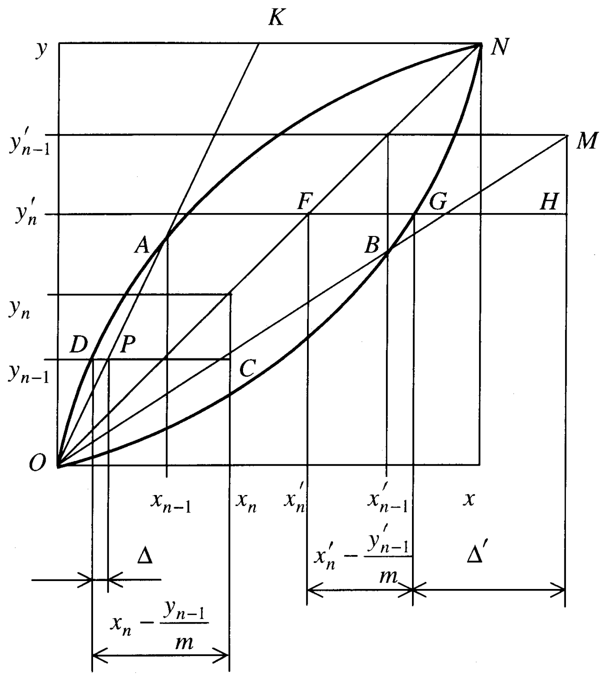

Fig. 1. Representation of the running equilibrium lines in the form of the straight lines $y = mx$.

highly volatile component as compared to the true value (segment *CD*), while the difference $x'_n - \frac{y'_{n-1}}{m}$ (segment *FH*) for the nonvolatile component turns out to be much more overstated (by Δ') as compared to the true value (segment *FG*). The employment of inaccurate values of the indicated or similar differences in computational procedures results in significant computational errors.

When formula (3) is employed, the running equations of equilibrium (see Fig. 2) for the *n*th plate are presented by the straight lines *AC* and *BD*, respectively, for the highly volatile and nonvolatile components. They are constructed in the form of tangents to the equilibrium curves at points *A* and *B* corresponding to the concentrations of the components after the plate x_{n-1} and x'_{n-1} and they cut off the segments *b* and *b*′, respectively, on the ordinate axis. In this case, the differences Δ and Δ' turn out to be close to the true values; consequently, formula (3) enables us to minimize computational errors.

The considered features of the complex model have been checked using the literature experimental data [9] on separation of the benzene–toluene mixture. The investigations were performed in the total-reflux regime in a column with three gauze-packing blocks above each of which distributors of the liquid were installed. The vapor moved horizontally within each step, and the motion of the vapor and liquid phases was a cross one. Because of the absence of experimental values for the concentrations of the vapor phase at the inlet and outlet of the upper section, we took them to be equal to the corresponding values in the liquid at the outlet and inlet of it since the composition of the vapor arriving at the dephlegmator is equal to the composition of the liquid coming out of it, and the rates of both flows are the same. The same reasoning was behind the selection of the composition of the vapor phase for the sections lying below. In the middle section, we obtained concentrations of the liquid which exceed the possibilities of one theoretical step, because of which the indices of this section have not been employed in analysis.

Using the data of [10] for the benzene–toluene mixture we have found the equilibrium dependence

$$y = \frac{1.35 - 0.1x}{0.58 + 0.67x}\,x\,, \tag{4}$$

in which the average deviation from the experimental data is no higher than ± 0.37%.

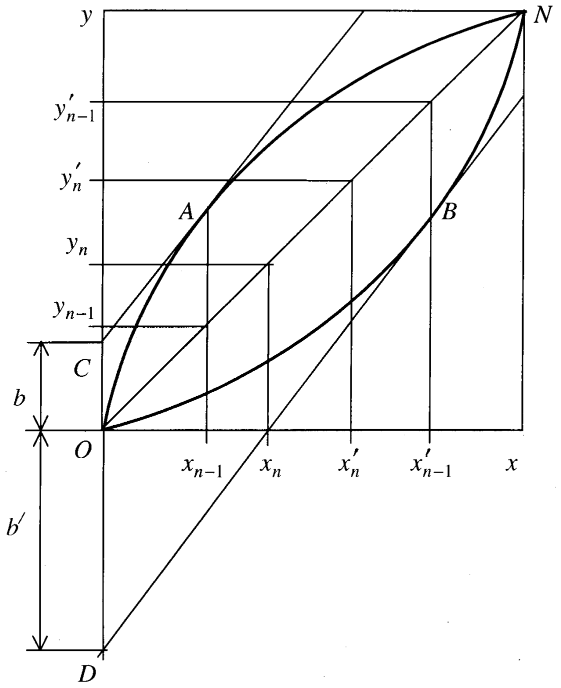

Fig. 2. Representation of the running equilibrium lines in the form of the tangent $y = ax + b$ to the equilibrium curve.

With allowance for $y' = 1 - y$ and $x' = 1 - x$, from (4) we have derived the relation for the nonvolatile component

$$y' = \frac{0.48 + 0.1x'}{1.25 - 0.67x'}x', \tag{5}$$

which holds with an accuracy no higher than 1.46%. In (4) and (5), the concentrations of the components in the liquid are presented in mole fractions.

It is known from [3] that the efficiency of mass exchange is determined from the formula

$$E_\text{k} = \frac{\frac{L}{mV} + 0.5 - h\frac{L}{mV} - h_1}{\frac{x_n - \frac{y_{n-1}}{m}}{x_n - x_{n-1}} - h\frac{L}{mV} - h_1}. \tag{6}$$

As a result of simultaneous solution of (1) and (6) with allowance for the features of the experimental data in question ($L = V$, $y_n = x_n$, and $y_{n-1} = x_{n-1}$) we have obtained

$$E_\text{k} = \frac{m\,(m+1)}{2\,(m^2 - 1)}\,\frac{x_n - x_{n-1}}{x_n}. \tag{7}$$

for the highly volatile component. Of analogous form is the formula for the nonvolatile component

$$E'_\text{k} = \frac{m'\,(m'+1)}{2\,[(m')^2 - 1]}\,\frac{x'_n - x'_{n-1}}{x'_n}. \tag{8}$$

TABLE 1. Results of the Calculation from Formulas (7) and (8)

x_n, %		x_{n-1}, %		m	m'	E_k	E_k'	$\frac{E_k - E_k'}{E_k}$, %
wt.	mol.	wt.	mol.					
Upper section								
54.5	58.56	49.0	53.13	1.3856	0.5629	0.1666	0.0844	49.35
63.0	66.76	58.4	62.35	1.2906	0.5188	0.1468	0.0716	51.24
67.2	70.73	65.5	69.13	1.2279	0.4897	0.0610	0.0262	56.96
58.3	62.25	52.5	56.59	1.3485	0.5457	0.1759	0.0900	48.81
Lower section								
17.9	20.46	16.5	18.19	1.8837	0.7940	0.0810	0.0377	53.49
30.9	34.53	26.1	29.41	1.6995	0.7085	0.1803	0.0952	47.21
28.0	31.45	23.5	26.60	1.7454	0.7299	0.1805	0.0956	47.06
24.2	27.36	21.8	24.75	1.7770	0.7445	0.1091	0.0524	52.02
30.5	34.11	24.4	27.57	1.7292	0.7224	0.2272	0.1290	43.20
37.1	41.23	29.3	32.83	1.6465	0.6740	0.2543	0.1504	40.88
21.3	24.20	18.4	21.01	1.8439	0.7755	0.1440	0.0727	49.52

Upon substitution of the experimental concentrations, the values of m and m' calculated from (4) and (5), and the relations $m = y/x$ and $m' = y'/x'$ in which the contents of the components in the liquid after the plate were employed, we have obtained in (7) and (8), respectively, the values of the efficiency given in Table 1.

As is seen in Table 1, the efficiencies determined for the highly volatile and nonvolatile components with the use of formula (2) differ by approximately a factor of 1.5. The error is affected not only by the difference of the concentrations on the plate but by the value of the concentration itself.

The slopes of the running equilibrium lines for Eq. (3) have been obtained from (4) and (5) as the corresponding derivatives

$$a = \frac{dy}{dx} = \frac{0.783 - 0.116x - 0.067x^2}{(0.58 + 0.67x)^2}\,, \tag{9}$$

$$a' = \frac{dy'}{dx'} = \frac{0.6 + 0.116x' + 0.067\,(x')^2}{(1.25 - 0.67x')^2}\,, \tag{10}$$

while the segments cut off by these straight lines on the ordinate axis have been obtained by simultaneous solution of (3), (4), and (6) and (3), (5), and (7)

$$b = \frac{0.9625x^2}{(0.58 + 0.67x)^2}\,, \tag{11}$$

$$b' = -\frac{0.3126 + 0.134x'}{(1.25 - 0.67x')^2}\,(x')^2\,. \tag{12}$$

With allowance for the methodology of [3], formula (6), $m = a$, and $m' = a'$ and for the above features of the experimental data in question, we have obtained the dependences for the highly volatile and nonvolatile components respectively:

TABLE 2. Results of the Calculation from Formulas (9)–(14)

x_n, mol.%	x_{n-1}, mol.%	a	a'	b	b'	E_{k}	E'_{k}	$\frac{E_{\mathrm{k}} - E'_{\mathrm{k}}}{E_{\mathrm{k}}}$, %
$x = x_{n-1}$								
Upper section								
58.56	53.13	0.8019	0.7638	0.3101	–0.0942	0.1122	0.1012	9.75
66.76	62.35	0.6877	0.6561	0.3759	–0.0517	0.0906	0.0799	11.85
70.73	69.13	0.6164	0.5901	0.4227	–0.0310	0.0326	0.0300	8.00
62.25	56.59	0.7564	0.7206	0.3351	–0.0759	0.1167	0.1034	11.39
Lower section								
20.46	18.19	1.5193	1.482	0.0689	–0.5548	0.0674	0.0688	–1.99
34.53	29.41	1.2307	1.1846	0.1379	–0.3361	0.1449	0.1475	–1.79
31.45	26.60	1.3001	1.2546	0.1184	–0.3852	0.1481	0.1534	–3.58
27.36	24.75	1.3487	1.3039	0.1060	–0.4209	0.0874	0.0885	–1.25
34.11	27.57	1.2754	1.2297	0.1251	–0.3674	0.1902	0.1998	–5.04
41.23	32.83	1.1527	1.1065	0.1621	–0.2838	0.2101	0.2136	–1.65
24.20	21.01	1.4546	1.4118	0.0818	–0.5026	0.1209	0.1270	–4.99
$x = x_n$								
Upper section								
58.56	53.13	0.7321	0.6977	0.3491	-0.0669	0.1034	0.0908	12.20
66.76	62.35	0.6403	0.6121	0.4065	-0.0374	0.0849	0.0736	13.32
70.73	69.13	0.6009	0.5759	0.4335	-0.0271	0.0318	0.0292	8.27
62.25	56.59	0.6888	0.6572	0.3752	-0.0521	0.1074	0.0926	13.81
Lower section								
20.46	18.19	1.4712	1.4288	0.0783	–0.5158	0.0654	0.0661	–0.97
34.53	29.41	1.1164	1.0704	0.1744	–0.2606	0.1333	0.1300	2.48
31.45	26.60	1.1835	1.1372	0.1522	–0.3040	0.1367	0.1356	0.76
27.36	24.75	1.2809	1.2352	0.1236	–0.3713	0.0834	0.083	0.52
34.11	27.57	1.1253	1.0792	0.1713	–0.2662	0.1718	0.1689	1.72
41.23	32.83	0.9908	0.9464	0.2217	–0.1863	0.1863	0.1744	6.36
24.20	21.01	1.3636	1.3189	0.1023	–0.4321	0.1143	0.1168	–2.19
$x = (x_n + x_{n-1})/2$								
Upper section								
58.56	53.13	0.7660	0.7297	0.3297	–0.0796	0.1080	0.0960	11.06
66.76	62.35	0.6635	0.6336	0.3912	–0.0441	0.0879	0.0768	12.64
70.73	69.13	0.6086	0.5830	0.4281	–0.0290	0.0322	0.0296	8.14
62.25	56.59	0.7216	0.6879	0.3552	–0.0632	0.1122	0.0980	12.70
Lower section								
20.46	18.19	1.4950	1.4532	0.0736	–0.5350	0.0664	0.0674	–1.48
34.53	29.41	1.1717	1.1255	0.1560	–0.2962	0.1395	0.1389	0.42
31.45	26.60	1.2399	1.1939	0.1352	–0.3425	0.1427	0.1447	–1.35
27.36	24.75	1.3142	1.2689	0.1147	–0.3954	0.0855	0.0858	–0.36
34.11	27.57	1.1972	1.1511	0.1480	–0.3132	0.1818	0.1845	–1.51
41.23	32.83	1.0677	1.0221	0.1917	–0.2307	0.1993	0.1940	2.64
24.20	21.01	1.4081	1.3643	0.0919	–0.4661	0.1178	0.1220	–3.58

$$E_{\mathrm{k}} = \frac{a\,(x_n - x_{n-1})}{2\left(\frac{a^2 - 1}{a + 1}\,x_n + b\right)}\,, \tag{13}$$

$$E'_{\mathrm{k}} = \frac{a'\,(x'_n - x'_{n-1})}{2\left[\frac{(a')^2 - 1}{a' + 1}\,x'_n + b'\right]}\,. \tag{14}$$

The results of the calculations from formulas (9)–(14) are given in Table 2. In (9)–(12), we have also used the data on the composition of the liquid after the plate as the running values of x.

Table 2 shows a satisfactory convergence of the efficiencies determined for the highly volatile and nonvolatile components. The deviations are smaller for lower values of the highly volatile component.

The use of the values x_n and $(x_n + x_{n-1})/2$ as the running concentrations of the components in the liquid in Eqs. (3) and (9)–(12) results in efficiencies slightly differing from the data which have been obtained upon the employment of the values x_{n-1} for this purpose (Table 2). The proximity of the calculation results, especially for one and the same plate, points to the fact that these errors, even if comparatively small, are most likely attributed to the inexactness of formulas (4) and (5) in which the deviation from the same experimental values is different. A comparison of the data of Table 2 shows that the average concentrations result in efficiencies and errors of their calculation for the highly volatile and nonvolatile components which are between the corresponding values obtained with the use of the compositions of the liquid at the beginning and at the end of the contact step.

The data of the table confirm, on the whole, the fact that it is possible to employ the complex model for calculation of the efficiency of mass exchange for both components. The use of formula (2) as the running equilibrium equation is adequate only for small differences of the compositions of the flows before and after the contact step, since otherwise we can have efficiencies or other calculated parameters much differing in the highly volatile and nonvolatile components. Unlike (2), expression (3) used for the same purpose enables us to obtain acceptable results irrespective of the values of the concentrations of the flows on the plate.

NOTATION

a, slope of the tangent to the equilibrium line; b, segment cut off on the ordinate axis by the tangent to the equilibrium line; E, efficiency of the plate; h and h_1, dimensionless distances from the site of injection of the vapor and the liquid, respectively, to the surface of equality of the concentrations of the phases on the ideal and real plates; L, molar flow of the liquid; m, coefficient of phase equilibrium; V, molar flow of the vapor; x and y, concentrations of the highly volatile components in the liquid and the vapor respectively. Subscripts: k, cross flow; n, No. of the plate in question; $n - 1$, No. of the preceding plate in the direction of vapor motion; $'$, nonvolatile component.

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