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PROCESSES AND EQUIPMENT OF CHEMICAL INDUSTRY

Analysis of Mass Exchange Efficiency in Rectifying Columns

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Abstract—Comparative analysis of the mass exchange efficiency at a complex simulation and at simulations of Murphree and Hausen was performed.

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Mass exchange simulations by Murphree [1] and Hausen [2] that differ in conditions of relation of ideal and real trays are used at the analysis of the process efficiency.

In Murphree models at the analysis of the efficiency in a vapor phase it was assumed that flows of an input vapor and of a liquid flowed down are equal by a composition and an amount, and at the analysis of the efficiency in a liquid phase concentrations and flows of the vapor leaving the trays and of the liquid feeding ones coincide. Whereas in the Hausen model the flows and compositions of the vapor, and the liquid feeding the both trays are equal.

The efficiency of the Murphree model is expressed by the following relations:

– in the vapor phase

$$E_{My} = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}}, \quad (1)$$

– in the liquid phase

$$E_{Mx} = \frac{x_n - x_{n-1}}{x_n - x_{n-1}^*} \quad (2)$$

where E is the mass exchange efficiency; x, y are concentrations of a volatile component in the liquid and vapor phases, respectively; M denote the Murphree model; n is the number of the considered tray; n–1 is the number of the underlying tray; x, y denote liquid and vapor flows, and * marks equilibrium conditions; y_n^* is the concentration of the vapor phase component after the tray being in equilibrium with the liquid leaving the tray; x_{n-1}^* is the concentration of the liquid phase component after the tray being in equilibrium with the vapor leaving the real tray.

In the general case the efficiencies E_{My} and E_{Mx} are not equal and that shows an ambiguity of the Murphree model.

Efficiencies relative to the vapor phase and the liquid in the Hausen model are equal

$$E_{Hy} = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}} = E_{Hx} = \frac{x_n - x_{n-1}}{x_n - x_{n-1}^*}, \quad (3)$$

where H denotes Hausen model.

The known models are visual since the mass exchange is depicted on a y–x chart. They are universal because they can be used for analysis of different mass exchange processes and equipments. However the Murphree and Hausen models assume full liquid agitation that in reality is observed rarely, and they do not consider engineering features of the processes. A neglect of these mass exchange features leads to narrowing a range of material properties, construction, and regime parameters where the calculated values of the efficiencies can be used. Thus employment of these models may result in the efficiency values that are more than unity or less than zero.

Other models that nevertheless are based on the known models with proper disadvantages are suggested for decreasing the negative consequences. In the developed complex models [3] a balance of the vapor and liquid

compositions on the real and ideal trays is assumed on some distance from the input point and not in the input or output points of the trays as in the known models. In [3, 4] it was assumed to determine this distance by a dependence on a coefficient of the phase equilibrium m. Such assumption adds dynamics to the new model since a character of the calculated relations depends on m and enables their use for device computation where the coefficient of the phase equilibrium is varied over steps of a contact. The Murphree and Hausen models in the compex model are taken into account as limit cases. The mass exchange efficiency in the complex model with respect to a direct flow is computed by the following equation:

$$E_{\mathrm{d}} = \frac{y_n - y_{n-1} + m\left(x_n - x_{n-1}\right)}{mx_n - y_{n-1} + x_{n-1} - \dfrac{y_n}{m}}, \qquad (4)$$

where m is the coefficient of the phase equilibrium, d denotes direct flow.

The comparative analysis of equations (1)–(4) shows that in the known models at least one of the concentrations of the volatile components in the liquid are required for the computation of the mass exchange efficiency in the vapor phase and one of the concentrations in the vapor phase for the computation of the mass exchange efficiency in the liquid. For example, the compositions of the vapor feeding the tray and leaving this tray and also of liquid flowing down from the contact step are required in equation (1) at the computation by the Murphree model. The composition of the components in the feeding liquid may vary in dependence on thermophysical properties of the interacting flows, construction features of an equipment, and regime parameters of the processes but in any case this does not affect the efficiency value.

The composition of the input and output liquid, and also of the vapor after the first contact step should be known for the use of equation (2). The composition of the components in the feeding vapor can vary in a wide range but this also does not affect the efficiency value. In the Hausen model the input and output concentrations of the both flows should be known at computation of the mass exchange efficiency by equation (3).

In the Hausen and complex models the compositions of the both flows before and after their interaction are required at computation of the efficiency by equations (3) and (4). Therefore indirectly the mass exchange features noted above can be taken into account. Then also from this point of view the new model may be considered as general in comparison with the known models.

Characteristics of the mixtures

Parameter	Ethanol–water	Furfural–water	Water–acetic acid
y_n, mole fraction	0.00645	0.00107	0.9784
y_{n-1}, mole fraction	0.00536	0.00096	0.9744
x_n, mole fraction	0.00106	0.00032	0.9781
x_{n-1}, mole fraction	0.00089	0.00029	0.9742
m	12.82	7.9	1.0083
E_{My}	0.1802	0.0826	0.5073
E_{Mx}	0.3053	0.1626	0.5030
E_{H}	0.3973	0.2213	0.6712
E_{d}	0.3794	0.2014	0.5061

The compositions and the efficiency for various mixtures computed by the equations (1)–(4) are listed in the table. As it is shown from this table the close values of the efficiency are obtained by the Hausen and complex models at the coefficients of the phase equilibrium that are significantly over unity for ethanol–water and furfural–water mixtures, and at $m \to 1$ for water–acetic acid mixture in the Murphree and complex models.

Such similarity of the values was noted also at computation of a direct flow-vortex contact element of main furfural and beer column of microbiologic manufactures [4, 5]. Hence the Hausen model can be applied at the large values of m, and the Murphree model at $m \to 1$. An employment of the known model can lead to significant errors at the engineering calculations since the coefficient of the phase equilibrium can change in the wide ranges over the trays of the column in dependence on the component concentration. Whereas use of the complex model gives applicable results.

Dependences of the mass exchange efficiencies in the considered models on the component concentration for the different mixtures are depicted in Figs. 1, 2. According to the Murphree model the efficiency values in the vapor phase are constant and equal to values in the table and in the liquid, also as the efficiencies in the

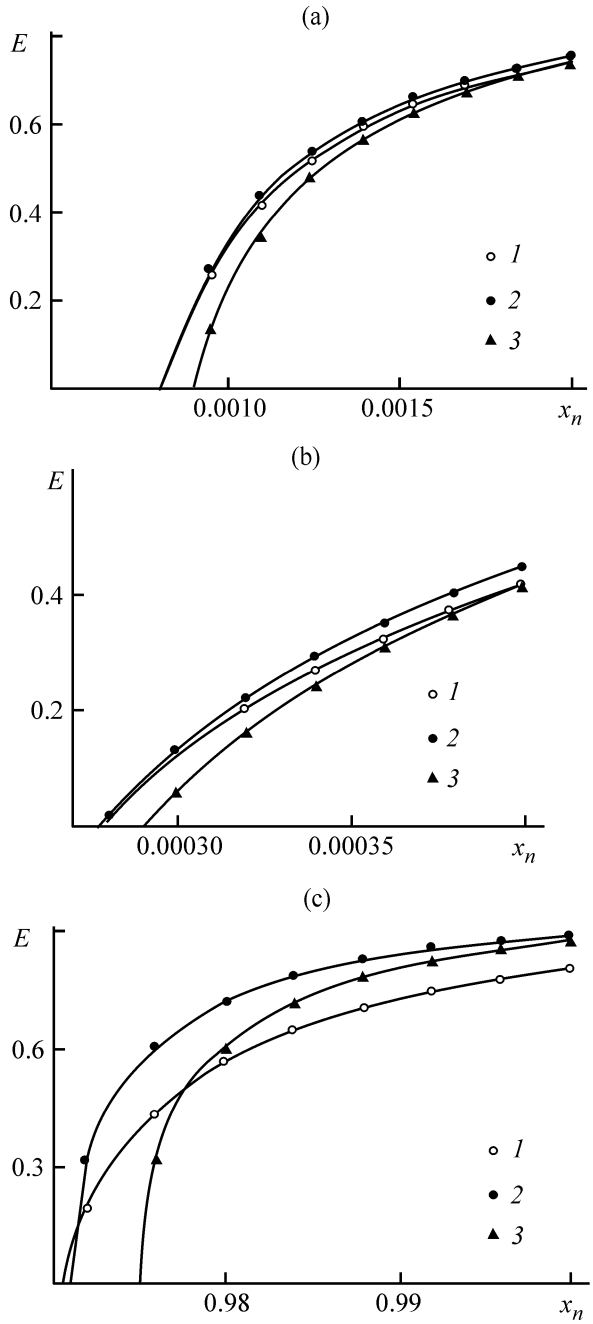

Fig. 1. Dependence of the efficiency E in the complex model (*1*), Hausen model (*2*), and Murphree model (relative to the liquid) (*3*) on the composition of the feeding liquid x_n (mole fraction) for the mixtures: (a) ethanol–water, (b) furfural–water, (c) water–acetic acid.

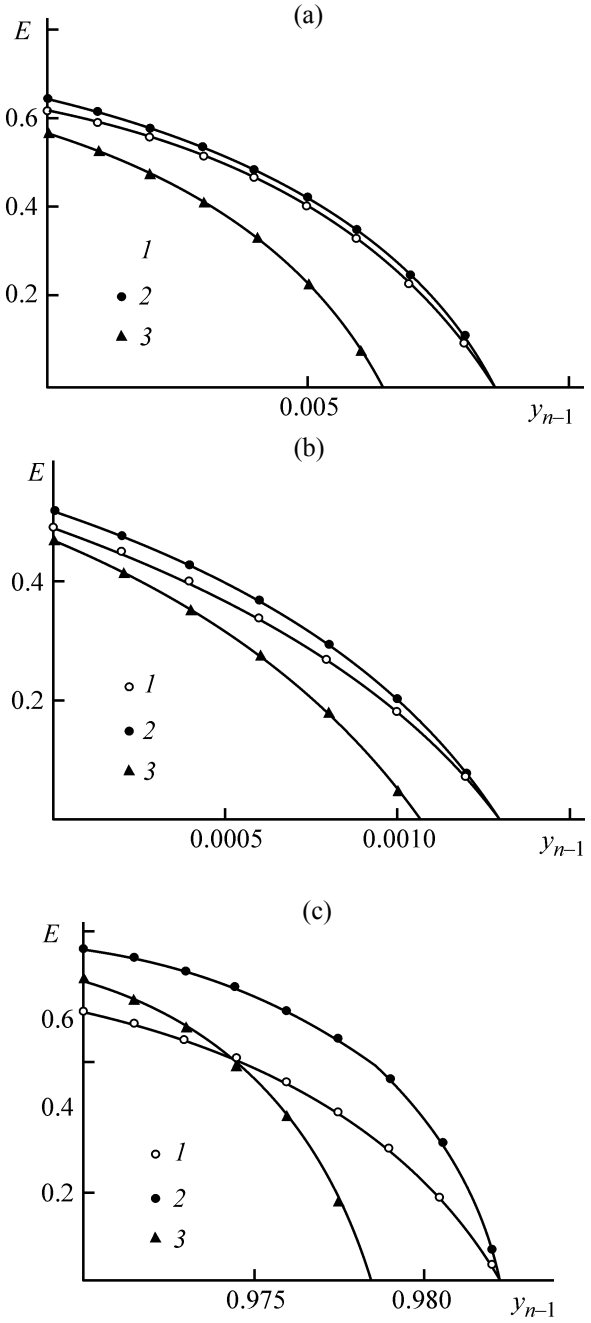

Fig. 2. Dependence of the efficiency E in the complex model (*1*), Hausen model (*2*), and Murphree model (relative to the vapor) (*3*) on the composition of the feeding vapor y_{n-1} (mole fraction) for the mixtures: (a) ethanol–water, (b) furfural–water, (c) water–acetic acid.

other models, vary in the wide ranges in the dependence on the composition of the feeding liquid lowering with a decrease in the liquid amount.

Such lowering of E at the decrease in y_{n-1} was depicted on Fig. 2 for the various models including the Murphree model at the analysis of the efficiency in the vapor phase while the efficiency in the liquid in the Murphree model are kept constant and that confirmed the disadvantages of the known model and its ambiguity.

Figures 1, 2 show also the closeness of the efficiency

in the complex model and of the Hausen model at $m >> 1$ (a, b) and their evident difference at $m > 1$ in the relatively wide range of the compositions of the feeding liquid and vapor (c).

At the change of the composition of the feeding vapor the mass exchange efficiency in the Murphree model significantly differs from the appropriate value of the complex model at the large coefficient of the phase equilibrium (Figs. 2a, 2b) and is equalized to it at the values of m tending to unity in the narrow range of y_{n-1} (Fig. 2c).

At the change of the composition of the feeding liquid the Murphree model is also close to the complex model in the narrow range of the liquid compositions for all considered mixtures (Fig. 1) thereby a difference of the efficiency values in this case is lesser essential than at the change of y_{n-1}.

CONCLUSIONS

The complex model can be used at the change of properties of the separated mixture, in particular at the change of the coefficient of the phase equilibrium, in the wide range while the known models are applicable in the narrow range of the properties.

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