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Modeling of rectification in a laboratory single-sieve tray column

D. R. Koleva[*], M. K. Karaivanova

Chemical Technologies Department, Technical Sciences Faculty, Prof. Dr Assen Zlatarov University, Burgas, Prof. Yakim Yakimov Blvd. 1, Burgas 8010, Bulgaria

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The design of rectification columns is based on the method of the "theoretical tray" and the actual setup of real-life trays is carried out with the help of various kinetic characteristics, such as tray efficiency. A theoretical method for calculating tray efficiency has not yet been proposed due to the complex hydrodynamic setting and the influence of a range of factors. Empirical correlations for calculating the local or integral efficiency of the tray can be found in the literature. The aim of the present work is to make a comparison between the experimentally obtained data from the rectification of a model tetrachloromethane-toluene binary mixture in a laboratory single-sieve tray column and the local efficiency data calculated by means of a model known from the literature, as well as to determine the parameters of the applied model. A good match was established between the calculated and experimental data about the local efficiency and the total number of mass-transfer units of the tetrachloromethane-toluene mixture, the maximum error being below ±25%. A match of the LPR% obtained by the model was found: with the percentage given when applying Zuiderweg's model (1982) and Chen and Chuang's model (1993) at HVC concentrations in the initial mixture 38.6% and 22.9%, respectively. The studied model can be used to predict the local efficiency in the rectification of any binary mixture depending on its physicochemical properties even at low vapor velocities.

Key words: distillation, sieve trays, local efficiency, number of mass-transfer units, percentage of liquid-phase resistance over total mass-transfer resistance

INTRODUCTION

Sieve tray columns are widely used in practice to separate liquid mixtures by means of rectification. Rectification tray columns are a kind of bubble apparatus where mass transfer between the two phases is carried out on trays located one above the other [1]. Optimizing distillation equipment and processes can improve both the profitability and the greenness of an operation [2]. One approach to optimizing distillation is to design green columns. As a more effective approach, Pilling and Summers [2] discussed to build columns with smart designs. The most important operating characteristics of a tray column are its performance (loads on both phases) and efficiency. The type and dimensions of the tray determine the working loads with regard to vapor and liquid at which it will most efficiently operate [3, 4].

The design of rectification columns is based on the method of the "theoretical tray", that is a tray where equilibrium concentrations of the interacting phases are assumed to occur. The actual setup of real trays is carried out with the help of different kinetic characteristics. One such characteristic is the tray efficiency. The efficiency of the mass exchange process on the individual tray is determined by the differential and integral characteristics [4]. The differential characteristics of mass-transfer efficiency (E_{OG}) depend on the kinetic parameters of the process and mainly reflect the diffusion resistances of the two contacting phases.

The initial studies of tray efficiency in rectification were based on the generalized experience gained in the operation of industrial columns and suggested empirical correlations for the calculation of the overall column efficiency or tray efficiency, especially of bubble cap and sieve trays. The first proposed correlations and their modifications were derived by summarizing the experience of operating rectification columns in the oil refining industry, where a small number of parameters affect the process (α, μ_L, x_F). Today, they are still used for initial calculation of the local efficiency in the separation of hydrocarbon mixtures.

Later, the proposed correlations included constructional and operating parameters, but remained valid only for a certain type of trays and operating conditions. Syeda and Afacan [5] reported a new model for predicting point efficiency of cross-flow sieve trays that has been developed based on the hydrodynamics of an operating sieve tray represented by the proposed froth structure model. This efficiency model is applicable for both froth

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[*] To whom all correspondence should be sent:
E-mail: *desikol@abv.bg*

and spray regime [5]. In work [6] appropriate ways are established for estimating the efficiencies of valve trays with downcomer and dualflow trays of industrial distillation columns. Different methods to predict the efficiency in valve trays and dualflow trays are developed and compared against data from three industrial distillation columns under different operating conditions [6, 7]. Lamprecht [8] focused on the development and experimental validation of two simplistic and cost-effective methods that can be used to quantify column internal efficiency. The ADIBAA (aqueous desorption of isobutyl acetate in air) and HA (humidification of air) methods are proposed for efficiency measurements in packed and tray columns, respectively [8, 9]. Chen and Chuang [10] have developed correlations for predicting the number of individual mass-transfer units and the liquid-phase resistance consistent with mass-transfer theories, and to compare the prediction with distillation data from commercial-size sieve tray columns.

The aim of the present work is to compare the local efficiency data obtained experimentally from rectification of a model tetrachloromethane-toluene binary mixture in a single-sieve tray laboratory column [11, 12] and the data calculated using a model known from the literature [10], as well as to determine the parameters of the applied model. The studied method is semi-empirical and allows for the calculation of the number of mass-transfer units and the local efficiency, as well as the determination of the percentage of the liquid phase resistance over the total resistance of the mass-transfer process. The present study is a continuation of the work of Karaivanova and Koleva [13].

Model structure

The differential (local or point) characteristic defines the mass transfer in an elementary volume of the gas-liquid system and the integral characteristic does so on the entire tray. The local efficiency coefficient, E_{OG}, (local efficiency) is used as a differential characteristic of the efficiency of mass transfer whilr the tray efficiency coefficient or Murphree efficiency, E_{MV}, is used as an integral characteristic of the mass transfer efficiency of the entire tray. By assuming that the flow rates are constant along the height of a counter-current column, we distinguish Murphree efficiency-E_{MV}, for the vapor phase of the nth tray as follows:

$$E_{MV} = \frac{y_n - y_{n-1}}{y^* - y_{n-1}}, \tag{1}$$

where: y_n, y_{n-1} are the average compositions of the outflowing and inflowing vapor flows on the nth tray, respectively; $y^*$is the composition of the vapors in equilibrium with the liquid outflowing from the tray with composition x_n.

To define the local (point) efficiency an analytical expression similar to equation (1) is used, the difference being that all concentrations refer to inflows and outflows of a randomly selected elementary volume of the gas-liquid layer. Thus, the vapor phase local efficiency will be determined by equation (2):

$$E_{OG} = \frac{y_p - y_{p-1}}{y^* - y_{p-1}}, \tag{2}$$

where p, p-1 refer to the inflows and outflows of an elementary volume.

Due to the complex hydrodynamic state and the influence of a number of factors, a theoretical method for calculating tray efficiency has not yet been proposed [13]. To determine the local efficiency, the model of Chen and Chuang [10] and a semi-empirical method for determining the model parameters were used. The studied semi-empirical method allows for the calculation of the local efficiency under the following assumptions and operating conditions [13]:

- The mass transfer mechanism on the dividing surface (interfacial area) between two phases is described by the Lewis and Whitman two-film theory. Mass transfer is regarded as a two-stage process of consecutive transfer of the substance through the liquid and vapor phases by molecular means. The dividing surface is assumed to have no resistance on the transfer, since a phase equilibrium between the concentrations of the transferred component in the two phases is established on it.
- The total resistance of the process is the sum of the resistances in the individual phases, with the distribution of the total resistance between the phases being also dependent on the phase equilibrium and the resistance through the dividing surface being zero.
- It is assumed that the transfer of the substance through a moving interfacial area is described by the penetration mechanism or the surface renewal mechanism.
- Ideal flow structures on the tray are assumed: a model of complete mixing of the liquid and a model of ideal (full) displacement for the vapor phase.
- Rectification is assumed to proceed under the conditions of total reflux (G = L) [13].

As a result of the above assumptions, the local efficiency calculation model was derived using the following scheme:

$$E_{OG} = 1 - exp(-N_{OG}) \tag{3}$$

$$N_{OG} = K_{OG}.a.t_G = \frac{N_G}{1+\lambda.\frac{N_G}{N_L}} = \frac{N_G}{1+m.\frac{G}{L}.\frac{N_G}{N_L}} \tag{4}$$

$$N_G = k_G.a.t_G = C_1.\frac{1}{\mu^{0.1}.\phi^{0,14}}.\left[\frac{F_S^2.\rho_L}{\sigma^2}\right]^{\frac{1}{3}}.\left(D_G.\grave{t}_G\right)^{0.5} \tag{5}$$

$$N_L = k_L.a.t_L =$$

$$C_2.\frac{1}{\mu^{0.1}.\phi^{0,14}}.\left[\frac{F_S^2.\rho_L}{\sigma^2}\right]^{\frac{1}{3}}.\left(\frac{M_G.G}{M_L.L}\right).\left(D_L.\grave{t}_L\right)^{0.5} \tag{6}$$

$$N_{OG} = \frac{N_G}{1+\lambda.\frac{N_G}{N_L}} = \frac{C_1.\frac{1}{\mu^{0.1}.\phi^{0,14}}.\left[\frac{F_S^2.\rho_L}{\sigma^2}\right]^{\frac{1}{3}}.\left(D_G.\grave{t}_G\right)^{0.5}}{\lambda.\frac{C_1}{C_2}.\left(\frac{D_G.\rho_G}{D_L.\rho_L}\right)^{0.5}.\left(\frac{M_L.L}{M_G.G}\right)+1} \tag{7}$$

The percentage of the liquid-phase resistance over the total mass-transfer resistance can be defined as:

$$LPR\% = \frac{\lambda/N_L}{1/N_G+\lambda/N_L} = \frac{m}{\frac{C_2}{C_1}.\left(\frac{D_L.\rho_L}{D_G.\rho_G}\right)^{0.5}.\left(\frac{M_G}{M_L}\right)+m} \tag{8}$$

where C_1, C_2 are the constants fitting by experimental data [11, 12].

In the model it is assumed that for the gas-liquid layer of the sieve tray, the time that the gas remains in the layer (holdup time) is equal to the contact time of the vapor phase in Higbie's model [13].

$$\theta_G = \frac{h_L}{W_V} = \grave{t}_G \tag{9}$$

$$\grave{t}_L = \frac{\grave{t}_G.\rho_L}{\rho_G} \tag{10}$$

The height of the clear liquid on the sieve tray plays an important role in the mass transfer process and is influenced by the holdup times of the vapor and liquid phases in the gas-liquid layer, t_G and t_L. In the present work, the height of the clear liquid on sieve trays was calculated using equation (11) proposed by Zuiderweg [14]:

$$h_L = 0,6.h_w^{0.5}.p^{0.25}.\left[\frac{(\rho_G/\rho_L)^{0.5}}{b}\right]^{0.25} \tag{11}$$

This allowed to determine the contact time in Higbie's model, which cannot be calculated or determined experimentally so far. The contact time for the liquid phase was calculated by the contact time of the vapor phase observing the condition that the two phases have equal volumetric flow rates.

The interfacial area was calculated using equation (12), proposed by Chen and Chuang [10].

$$a = \frac{1}{\mu^{0.1}.\phi^{0.14}}.\left[\frac{F_S^2.\rho_L}{\sigma^2}\right]^{\frac{1}{3}} \tag{12}$$

$$F_s = W_V.(\rho_G)^{0.5} \tag{13}$$

To compare the experimentally obtained local efficiency data and the data calculated by the model, a model tetrachloromethane-toluene binary mixture was chosen. The experiments were carried out using a laboratory single-sieve tray glass column with a diameter of 0.032 m and external outlet weirs [12]. The small diameter of the column and the outlet weirs ensured the inflow of the liquid for complete mixing on the tray and allowed for a direct experimental determination of the local efficiency. For complete mixing of the liquid on the tray and full displacement of the vapor phase in height of the gas-liquid layer, the two efficiencies have the same values [13]:

$$E_{MV} = E_{OG} \tag{14}$$

To determine the experimental number of mass-transfer units in rectification, the following dependence was used:

$$N_{OG-exp} = -ln\left(1 - E_{OG-exp}\right) \tag{15}$$

Equation (1) was used to determine the experimentally obtained local efficiency E_{OG-exp}.

RESULTS AND DISCUSSION

Constants C_1 and C_2 of the model were determined under the conditions of total reflux G/L = 1 from equation (7) by using experimental data for N_{OG}, as a function of the slope of the equilibrium line m by the following equations:

$$N_{OG-cal} = \frac{C_1.A}{m.z_1.B+1} \tag{16}$$

$$A = \frac{1}{\mu^{0.1}.\phi^{0,14}}.\left[\frac{F_S^2.\rho_L}{\sigma^2}\right]^{\frac{1}{3}}.\left(D_G.\grave{t}_G\right)^{0.5} \tag{17}$$

$$B = \left(\frac{D_G.\rho_G}{D_L.\rho_L}\right)^{0.5}.\left(\frac{M_L.L}{M_G.G}\right) \tag{18}$$

$$z_1 = C_1/C_2 \tag{19}$$

The values of the constants obtained for the tetrachloromethane-toluene model mixture were published in [13].

Fig. 1. Comparison between the experimental data on the local efficiency for the tetrachloromethane-toluene mixture and those calculated by the model.

Fig. 1 shows a comparison between the experimentally obtained data on the local efficiency and those calculated by the model. For the tetrachloromethane-toluene mixture, the applied model enabled the prediction of the local efficiency by vapor phase, in this case, with a maximum error below $\pm 25\%$ compared to that obtained experimentally.

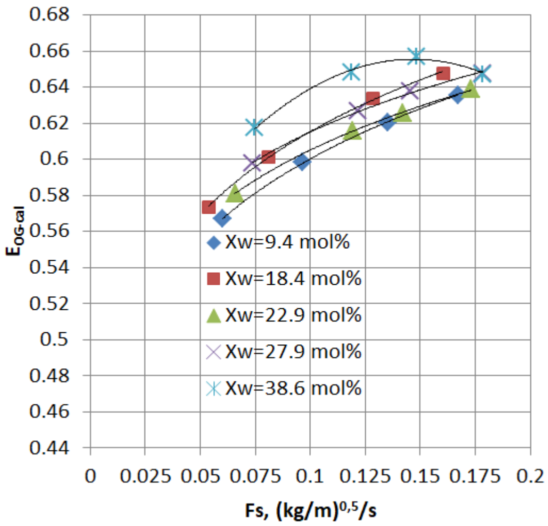

Fig. 2. Dependence of E_{OG-cal} calculated by equation (3) on the load factor (F-factor) at HVC concentrations of the initial mixture of 9.4%; 18.4%; 22.9%; 27.9% and 38.6%.

For the studied tetrachloromethane-toluene mixture, the range of the load factor is $F_s = 0.05 \div 0.18$ kg$^{0.5}$/(m$^{0.5}$.s) at vapor velocity $W_V = 0.0288 \div 0.0874\ m/s$ at concentrations of highly volatile components (HVC) in the initial mixture of 9.4%; 18.4%; 22.9%; 27.9% and 38.6%. As can be seen from Fig. 2, the increase of the load factor leads to an increase of the local efficiency calculated by the model and it reaches 66% at a load factor of 0.15 kg$^{0.5}$/(m$^{0.5}$.s) at HVC concentration of the initial mixture of 38.6%.

When the load factor changes in the interval $F_s = 0.075 \div 0.16$ kg$^{0.5}$/(m$^{0.5}$.s), there is a coincidence of the local efficiency E_{OG-cal} calculated by the model at HVC concentrations of the initial mixture of 18.4% and 27.9 %. The values of the local efficiency E_{OG-cal} calculated by the model also coincide in the load factor interval $F_s = 0.125 \div 0.175$ kg$^{0.5}$/(m$^{0.5}$.s) at HVC concentrations of the initial mixture of 9.4% and 22.9% (Fig. 2).

The dependence of the number of vapor phase mass-transfer units N_{G-cal} on the flow parameters under total reflux conditions is shown in Fig. 3.

In a narrow range of variation of the flow parameters there is an increase from 1 to 1.04 in the number of mass-transfer units by vapor phase calculated by the model. There is little research in the literature on this small interval of flow parameters $FP = 0.0576 \div 0.0604$ corresponding to low vapor velocities. For the tetrachloromethane-toluene mixture studied, a coincidence of the number of mass-transfer units per vapor phase N_{G-cal} calculated by equation (16) with those of Zuiderweg [14] is observed when FP changes from 0.0576 to 0.0604 (Fig. 3).

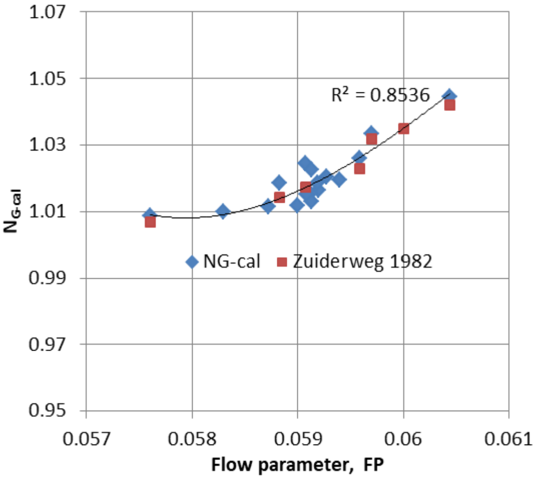

Fig. 3. Comparison between the number of vapor phase mass-transfer units N_{G-cal} with results of [14].

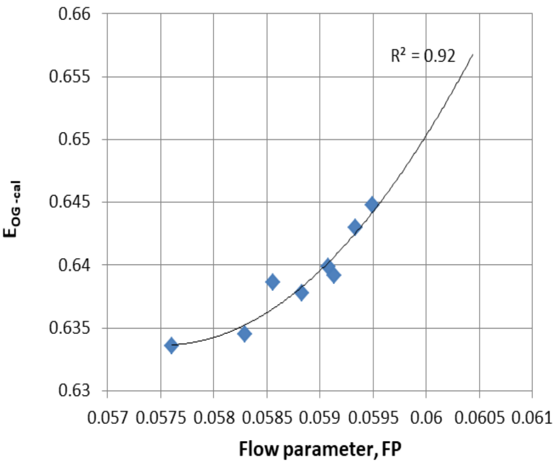

Fig. 4. Effect of the flow parameters under total reflux conditions (FP) on the vapor phase local efficiency calculated by the model, E_{OG-cal}.

With the increase of HVC concentration in the initial mixture from 22.9%; 27.9% to 38.6% and changes in the flow parameters in the interval $FP = 0.0576 \div 0.0595$, corresponding to vapor velocity $W_V = 0.0705 \div 0.088\ m/s$, a smooth increase in the local efficiency by vapor phase calculated by the model E_{OG-cal} can be seen, the maximal error being below $\pm 25\%$ (Fig. 4).

The applied model also allows the prediction of the total number of mass-transfer units, in this case by vapor phase, at maximum error below 25%, as compared to those obtained in the tetrachloromethane-toluene mixture experiment (Fig. 5).

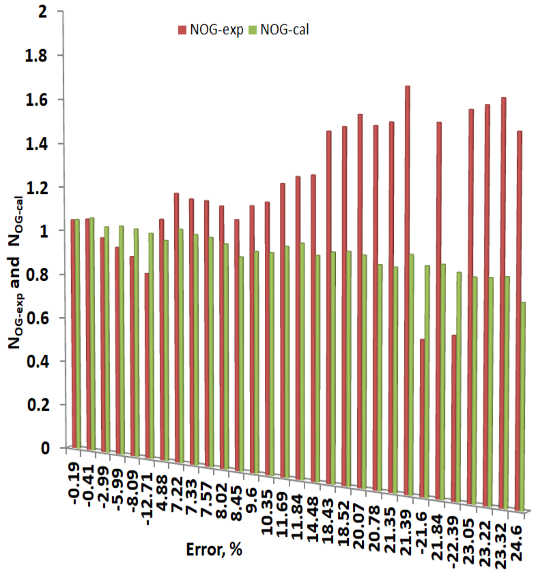

Fig. 5. Comparison between the experimental data on the total number of mass-transfer units for the tetrachloromethane-toluene mixture and those calculated by the model.

Porter and Jenkins [15] pointed out that under the conditions of total reflux all properties of a system can be expressed as a function of the flow parameters $FP = \left(\frac{\rho_G}{\rho_L}\right)^{0.5}$. The flow parameters can be used as a variable to compare the local efficiency, the number of transfer units in the mass-exchange process, the resistance of the liquid phase on the total resistance of the mass-transfer process and to predict them by existing models.

Fig. 6 shows a match of the LPR% obtained by the applied model for the tetrachloromethane-toluene mixture at a concentration of HVC in the initial mixture of 38.6% with the percentage given by applying Zuiderweg's model [14] and, at a concentration of HVC in the initial mixture of 22.9%, with those presented by applying Chen and Chuang's model [10]. The match of the LPR% values obtained by the applied model with those presented by Zuiderweg [14] and Chen and Chuang [10] corresponds to a variation of the flow parameters $FP = 0.0580 \div 0.0596$. For a small range of flow parameters Chen and Chuang's FP model [10] gives high LPR% values compared to other models. For the studied mixture, higher LPR% values were obtained compared to Chen and Chuang's model [10] at an HVC concentration in the initial mixture of 9.4% for LPR% from 61% to 68% and at an HVC concentration in the initial mixture of 18.4% for LPR% from 70.1% to 70.8% (for variation of flow parameters $FP = 0.0586 \div 0.0604$). LPR% values of 47.8% to 56.2% were obtained at an HVC concentration in the initial mixture of 27.9% in a narrow variation range of the flow parameters $FP = 0.0581 \div 0.0596$ (Fig. 6).

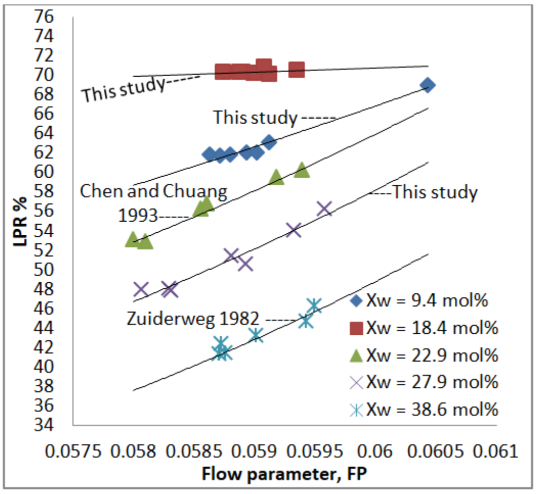

Fig. 6. Comparison of the resistance of the liquid phase over the total resistance of the mass-transfer process, LPR% for the tetrachloromethane-toluene mixture with that obtained by other models.

CONCLUSIONS

The feasibility of a semi-empirical model developed on the basis of Lewis and Whitman's model and the penetration model for calculating the local efficiency for a tetrachloromethane-toluene model mixture was checked. The values of the constants in the model were determined, based on a comparison between the experimentally obtained local efficiency data and those calculated by the model. A good match was established between the calculated and experimental data about the local efficiency and the total number of mass-transfer units of the tetrachloromethane-toluene mixture, the maximum error being below ±25%. For the studied mixture, a match of the number of mass-transfer units by vapor phase calculated by the model with those of Zuiderweg [14] was found for FP from 0.0576 to 0.0604. With the increase of HVC concentration in the initial mixture from 22.9% to 38.6% and changes in the flow parameters in the interval $FP = 0.0576 \div 0.0595$, corresponding to vapor velocity $W_V = 0.0705 \div 0.088\, m/s$, a smooth increase in the local efficiency by vapor phase calculated by the model was established, the maximal error being below $\pm$ 25%. A match of the LPR% obtained by the model was found: with the percentage given when applying Zuiderweg's model [14] at an HVC concentration in the initial mixture of 38.6%, and with the percentage presented when applying Chen and Chuang's model [10] at an HVC concentration in the initial mixture of 22.9%. Higher LPR% values were obtained compared to Chen and Chuang's model [10]: LPR% from 61 to 68% at an HVC concentration in the initial mixture of 9.4% and LPR% from 70.1 to 70.8% at an HVC concentration in the initial mixture of 18.4%. The studied model can be used to predict the local efficiency in the rectification of any binary mixture depending on its physicochemical properties even at low vapor velocities.

Nomenclature

N_{OG}, N_G, N_L – number of overall vapor-phase mass-transfer units, number of vapor-phase units, number of liquid phase mass-transfer units;

$K_{OG}.a, k_G.a, k_L.a$ – overall volume mass-transfer coefficient, vapor phase volume mass-transfer coefficient, liquid phase volume mass-transfer coefficient, s^{-1};

$\lambda = \frac{m.G}{L}$ – diffusion potential;

m – slope of vapor-liquid equilibrium line;

G and L – vapor and liquid flow rate, kmol/s;

K_{OG}, k_G, k_L - overall mass-transfer coefficient based on vapor, vapor-phase, and liquid-phase mass-transfer coefficients, m/s;

a – interfacial area per unit volume of two-phase dispersion m^2/m^3;

t_G, t_L - holdup time of vapor and liquid phases in the gas-liquid layer, s;

C_1, C_2 – constants in the studied model determined by processing experimental and calculated data;

θ_G – contact time, time that each elementary vapor volume spends on the interfacial area, s;

h_L – clear liquid height on a sieve tray, m;

$LPR\%$ - the percent of liquid-phase resistance over total mass-transfer resistance;

h_W – outlet weir height, m;

p –pitch of holes in a sieve tray, m;

ρ_G, ρ_L – vapor and liquid phase densities, kg/m^3;

b – length of overflow threshold per unit working (bubbling) area of the tray, m^{-1};

W_V – vapor velocity relative to the working area of the tray, m/s;

F_s – load factor, Fs = superficial F-factor, $kg^{0.5}/(m^{0.5}.s)$;

ϕ – fractional perforated tray area;

σ – surface tension, N/m^2;

A and B – variables calculated using equations (17) and (18), respectively;

FP – flow parameter under total reflux conditions $FP = \left(\frac{\rho_G}{\rho_L}\right)^{0.5}$

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