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RESEARCH ARTICLE

A MODEL FOR PREDICTING THE NUMBER OF MASS-TRANSFER UNITS AND THE EFFICIENCY OF SIEVE TRAYS IN RECTIFICATION

Mariana Karaivanova and Desislava Koleva

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Abstract

The design of rectification columns is based on the method of the "theoretical tray" and the actual setup of real trays is carried out with the help of various kinetic characteristics, such as tray efficiency. The relation between local and integral efficiency is a complex function of geometric, physicochemical and hydrodynamic factors. A theoretical method for calculating the tray efficiency has not yet been proposed, because of the complex hydrodynamic setting and the influence of a number 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 calculated local efficiency data by means of a model known from the literature and the experimentally obtained data from the rectification of a model Tetrachloromethane-Toluene binary mixture in a laboratory single-sieve tray column. Among the tasks of the current work is also to determine the parameters of the applied model. The proposed method is semi-empirical and allows for the calculation of the number of mass-transfer units and, therefore, of the local efficiency.

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Introduction:-

The most important operating characteristics of a tray rectification column are its performance (loads by both phases) and efficiency. The type and dimensions of the tray determine the working loads with regards to vapour and liquid with which it will operate with high efficiency [1, 2].

The design of rectification columns is based on the method of the "theoretical tray" and the actual setup of real trays is carried out with the help of different kinetic characteristics, one of them being tray efficiency. The differential and integral characteristics determine the efficiency of the mass exchange process on the individual tray [1÷3]. The local efficiency coefficient, E_{OG} , (local efficiency) is used as a differential characteristic of the efficiency of mass transfer and the tray efficiency coefficient or Murphree efficiency, E_{MV} , is used as an integral characteristic of the mass transfer efficiency of the entire tray. The differential (local) characteristic determines the mass transfer in an elementary volume of the gas-liquid system and the integral does so on the entire tray. By assuming that the flow rates are constant along the height of a countercurrent column, we distinguish Murphree efficiency, E_{MV} , for the vapour phase of the n^{th} tray as follows [4÷6]:

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

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

Local efficiency is defined by an analytical expression similar to equation (1), except that all concentrations refer to inflows and outflows of a randomly chosen elementary volume of the gas-liquid layer. Then, the vapour phase local efficiency will be determined from equation (2) [4÷6]:

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

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

The local characteristics of mass-transfer efficiency (E_{OG}) depend on the kinetic parameters of the process and reflect mainly the diffusion resistances of the two contacting phases. The study of tray efficiency in rectification was initially based on the summed-up experience gained in the operation of industrial towers and the suggestion of empirical correlations for the calculation of the overall column efficiency or tray efficiency of bubble cap and sieve trays [1÷6].

The first proposed correlations and their modifications were derived by summarizing the experience of operation of rectification columns in oil refining, where there are a small number of parameters affecting 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 constructive and operating parameters, but remained valid only for a certain type of trays and operating conditions [7, 8].

The present work aims to compare local efficiency data calculated using a model known from the literature [9] and experimentally obtained data from rectification of a model Tetrachloromethane-Toluene binary mixture in a single-sieve tray laboratory column [10, 11]. Among the tasks of the study is also 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, therefore, of the local efficiency.

Model structure

As is known, tray efficiency has to be known in order to take a step from the theoretically calculated trays to the number of actual trays. Due to the complex hydrodynamic state and the influence of a number of factors, a theoretical method for calculating the tray efficiency has not yet been proposed. To determine the local efficiency, the model of Chen and Chuang (1993) and a semi-empirical method for determining the model parameters are used. This semi-empirical method allows for the calculation of the local efficiency under the following assumptions and operating conditions:

1. 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 vapour 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.
2. 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.
 - a. 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.
 - b. 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.
3. *Rectification is assumed to proceed under the conditions of total reflux ($G = L$).

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

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

$$N_{OG} = K_{OG} \cdot a \cdot t_G = \frac{N_G}{1 + \lambda \frac{N_G}{N_L}} = \frac{N_G}{1 + m \frac{G}{L} \frac{N_G}{N_L}} \quad (4)$$

$$N_G = k_G \cdot a \cdot t_G = C_1 \cdot \frac{1}{\mu^{0.1} \cdot \phi^{0.14}} \cdot \left[\frac{F_S^2 \cdot \rho_L}{\sigma^2} \right]^{\frac{1}{3}} \cdot (D_G \cdot t_G)^{0.5} \quad (5)$$

$$N_L = k_L \cdot a \cdot t_L = C_2 \cdot \frac{1}{\mu^{0.1} \cdot \phi^{0.14}} \cdot \left[\frac{F_S^2 \cdot \rho_L}{\sigma^2} \right]^{\frac{1}{3}} \cdot \left(\frac{M_G \cdot G}{M_L \cdot L} \right) \cdot (D_L \cdot t_L)^{0.5} \quad (6)$$

$$N_{OG} = \frac{N_G}{1 + \lambda \frac{N_G}{N_L}} = \frac{C_1 \cdot \frac{1}{\mu^{0.1} \cdot \phi^{0.14}} \cdot \left[\frac{F_S^2 \cdot \rho_L}{\sigma^2} \right]^{\frac{1}{3}} \cdot (D_G \cdot t_G)^{0.5}}{\lambda \cdot \frac{C_1}{C_2} \cdot \left(\frac{D_G \cdot \rho_G}{D_L \cdot \rho_L} \right)^{0.5} \cdot \left(\frac{M_L \cdot L}{M_G \cdot G} \right) + 1} \quad (7)$$

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

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

where C_1 , C_2 are constants in the model.

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 vapour phase in Higbie's model.

$$\theta_G = \frac{h_L}{W_V} = t_G(9); \quad t_L = \frac{t_G \cdot \rho_L}{\rho_G} \quad (10)$$

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 . This allows to determine the contact time in Higbie's model, which has not been calculated or determined experimentally so far. The contact time for the liquid phase is calculated by the contact time of the vapour phase observing the condition that the two phases have equal volumetric flow rates.

To achieve the objectives of the present work, the 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 with external outlet weirs [11]. The small diameter of the column and the outlet weirs ensure the inflow of the liquid for complete mixing on the tray and allows for a direct experimental determination of the local efficiency. For complete mixing of the liquid on the tray and a full displacement of the vapour phase in height of the gas-liquid layer, the two efficiencies have the same values:

$$E_{MV} = E_{OG} \quad (11)$$

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

$$N_{OG-exp} = -\ln(1 - E_{OG-exp}) \quad (12)$$

Equation (1) was used to determine the experimentally determined 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 by the following equations:

$$N_{OG-cal} = \frac{C_1 \cdot A}{m \cdot z_1 \cdot B + 1} \quad (13)$$

$$A = \frac{1}{\mu^{0.1} \cdot \phi^{0.14}} \cdot \left[\frac{F_S^2 \cdot \rho_L}{\sigma^2} \right]^{\frac{1}{3}} \cdot (D_G \cdot t_G)^{0.5} \quad (14)$$

$$B = \left(\frac{D_G \cdot \rho_G}{D_L \cdot \rho_L} \right)^{0.5} \cdot \left(\frac{M_L \cdot L}{M_G \cdot G} \right) \quad (15)$$

$$z_1 = C_1/C_2 \quad (16)$$

The values of the constants obtained for the Tetrachloromethane-Toluene model mixture were: $C_1 = 11$ and $C_2 = 14$.

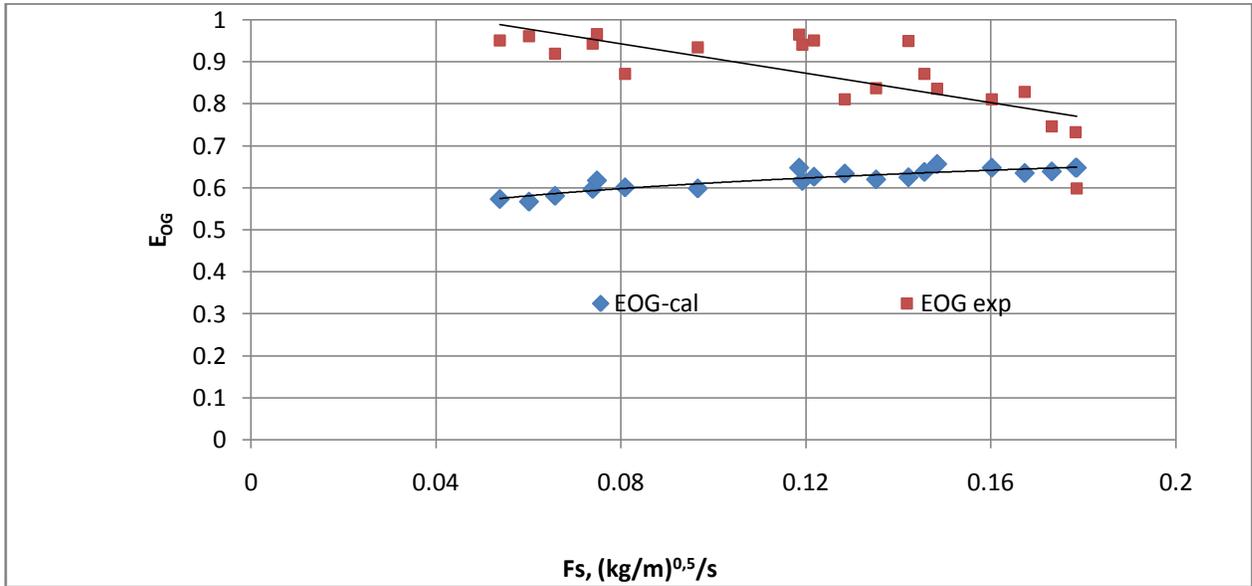


Fig. 1:- Dependence of the experimentally determined local efficiency E_{OG-exp} and the efficiency calculated by the model E_{OG-cal} on the load factor, F-factor.

For the studied Tetrachloromethane-Toluene mixture the load factor range was $F_s = 0.05 \div 0.18 \text{ kg}^{0.5}/(\text{m}^{0.5}.\text{s})$ at concentrations of highly volatile components (HVC) in the initial mixture of 9.4%; 18.4%; 22.9%; 27.9% and 38.6%. With the increase of the load factor the experimental local efficiency E_{OG-exp} decreased from 96% to 73% and the calculated local efficiency increased from 57% to 66% (Fig. 1). In the load factor variation interval $F_s = 0.05 \div 0.11 \text{ kg}^{0.5}/(\text{m}^{0.5}.\text{s})$, corresponding to a vapour velocity $W_v = 0.0288 \div 0.0692 \text{ m/s}$, the values of the calculated local efficiency E_{OG-cal} were smaller than those of the experimental local efficiency E_{OG-exp} , with a maximum error under $\pm 35\%$ (Fig. 1).

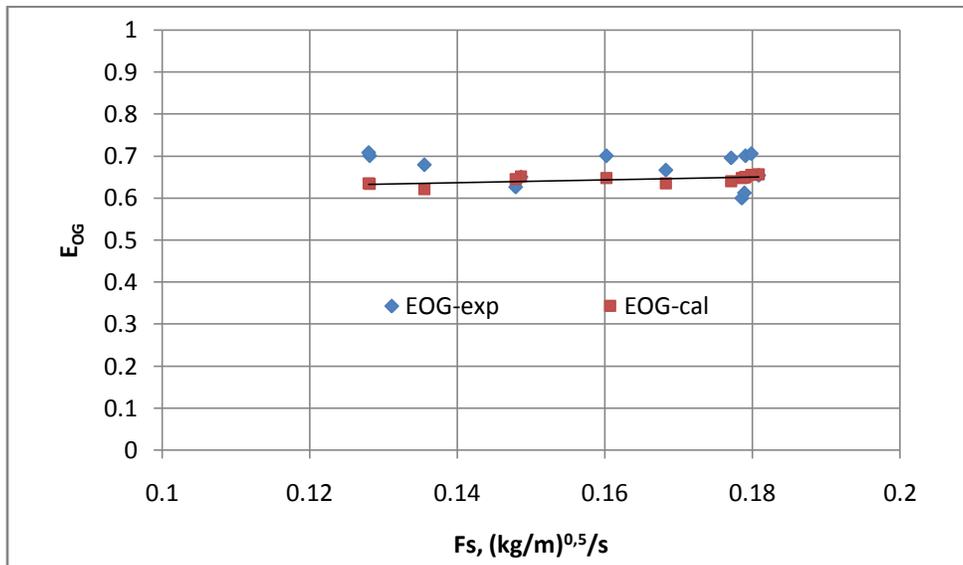


Fig. 2:- Dependence of the experimentally determined local efficiency E_{OG-exp} and the efficiency calculated by the model E_{OG-cal} on the load factor, F-factor.

As Fig 2 shows, when vapour velocity W_V increased from 0.0692 to 0.0874 m/s, corresponding to a load factor in the range $F_s = 0.12 \div 0.18 \text{ kg}^{0.5}/(\text{m}^{0.5} \cdot \text{s})$, E_{OG-cal} and E_{OG-exp} matched well with a maximum relative error under $\pm 25\%$. This means that for a load factor $F_s = 0.12 \div 0.18 \text{ kg}^{0.5}/(\text{m}^{0.5} \cdot \text{s})$ for the Tetrachloromethane-Toluene mixture the applied model is capable of predicting the local efficiency, in this case by vapour phase, matching the experimental data with a maximum error below $\pm 25\%$.

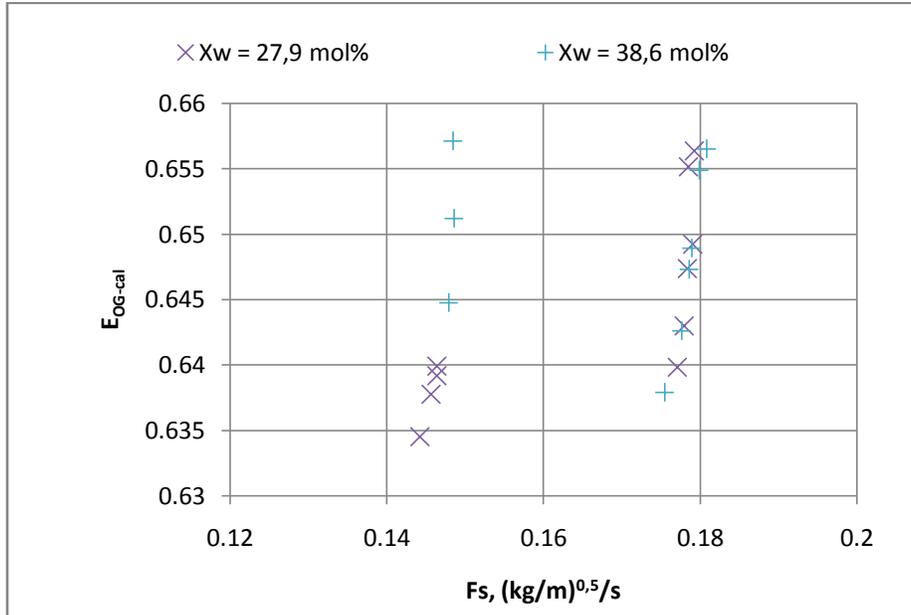


Fig. 3:- Dependence of the efficiency calculated by the model E_{OG-cal} on the load factor, F-factor at HVC concentrations of the initial mixture of 27.9% and 38.6%.

At a load factor in a narrow range $F_s = 0.17 \div 0.18 \text{ kg}^{0.5}/(\text{m}^{0.5} \cdot \text{s})$ for HVC concentrations in the initial mixture of 27.9% and 38.6%, the values of the local efficiency E_{OG-cal} calculated by the model coincide (Fig. 3).

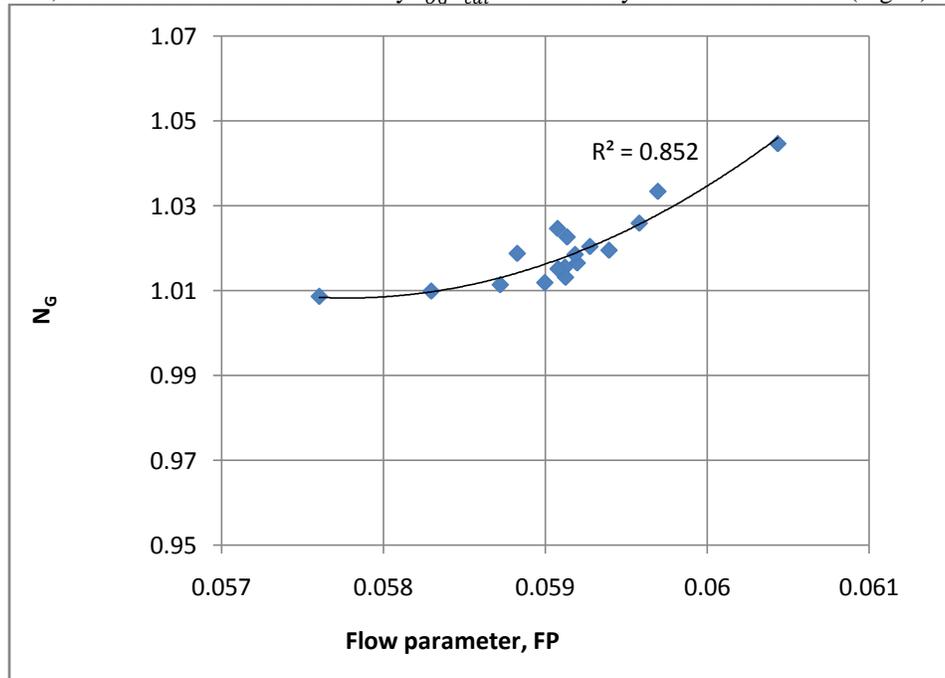


Fig. 4:- Dependence of the number of vapour phase mass-transfer units N_{G-cal} on the flow parameters, FP.

The dependence of the number of vapour phase mass-transfer units N_{G-cal} on the flow parameters under the conditions of total reflux is shown in Fig. 4. For the studied Tetrachloromethane-Toluene mixture, in a narrow variation range of the flow parameters there was an increase in the number of vapour phase mass-transfer units from 1 to 1.04 calculated by the applied model (equation (13)). There is little research in the literature on this small variation range of the flow parameters $FP = 0.0576 \div 0.0604$ corresponding to low vapour velocities (Fig. 4).

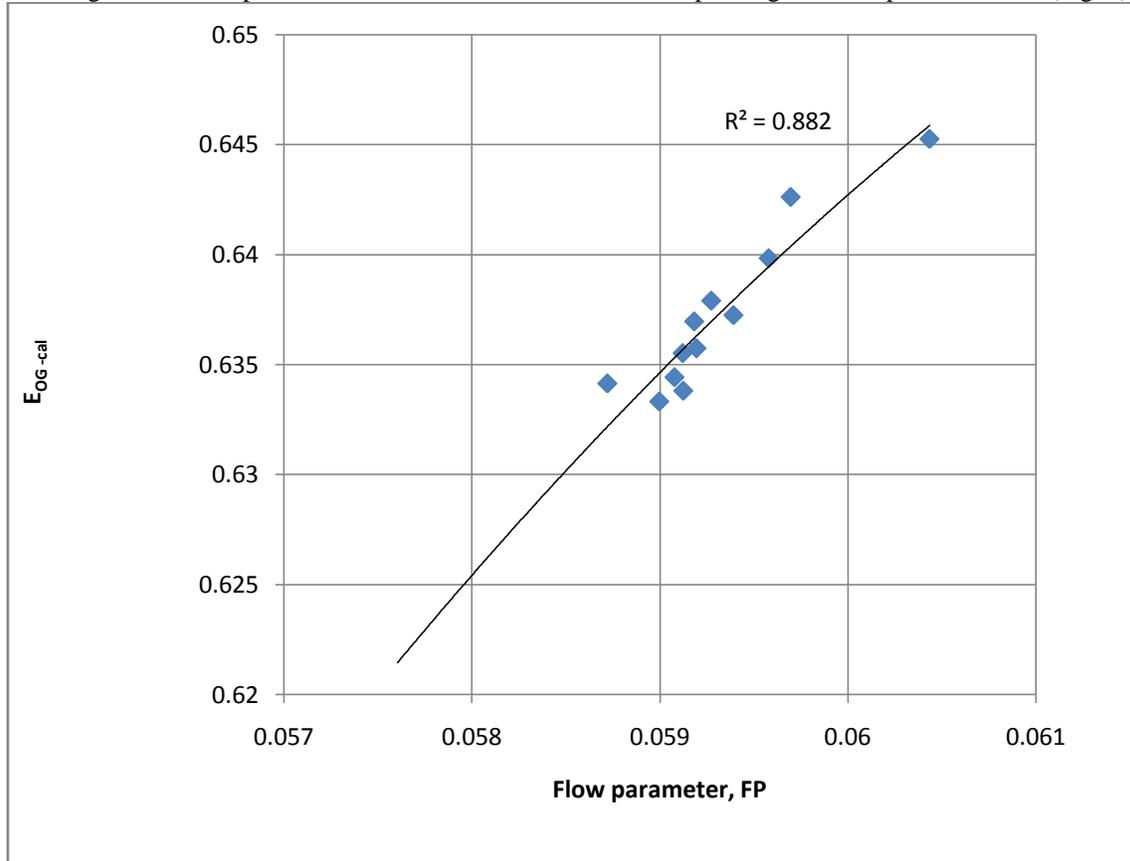


Fig. 5:- Dependence of the flow parameters (FP) under the conditions of total reflux on the vapour phase local efficiency calculated by the model E_{OG-cal} .

When the flow parameters change in the range $FP = 0.059 \div 0.0605$, corresponding to vapour velocity $W_V = 0.0692 \div 0.088 \text{ m/s}$, there was a linear increase of the vapour phase local efficiency calculated by the model E_{OG-cal} , with a maximum error below $\mp 25\%$ for HVC concentrations in the initial mixture of 9.4%; 18.4%; 22.9%; 27.9% and 38.6% (Fig. 5).

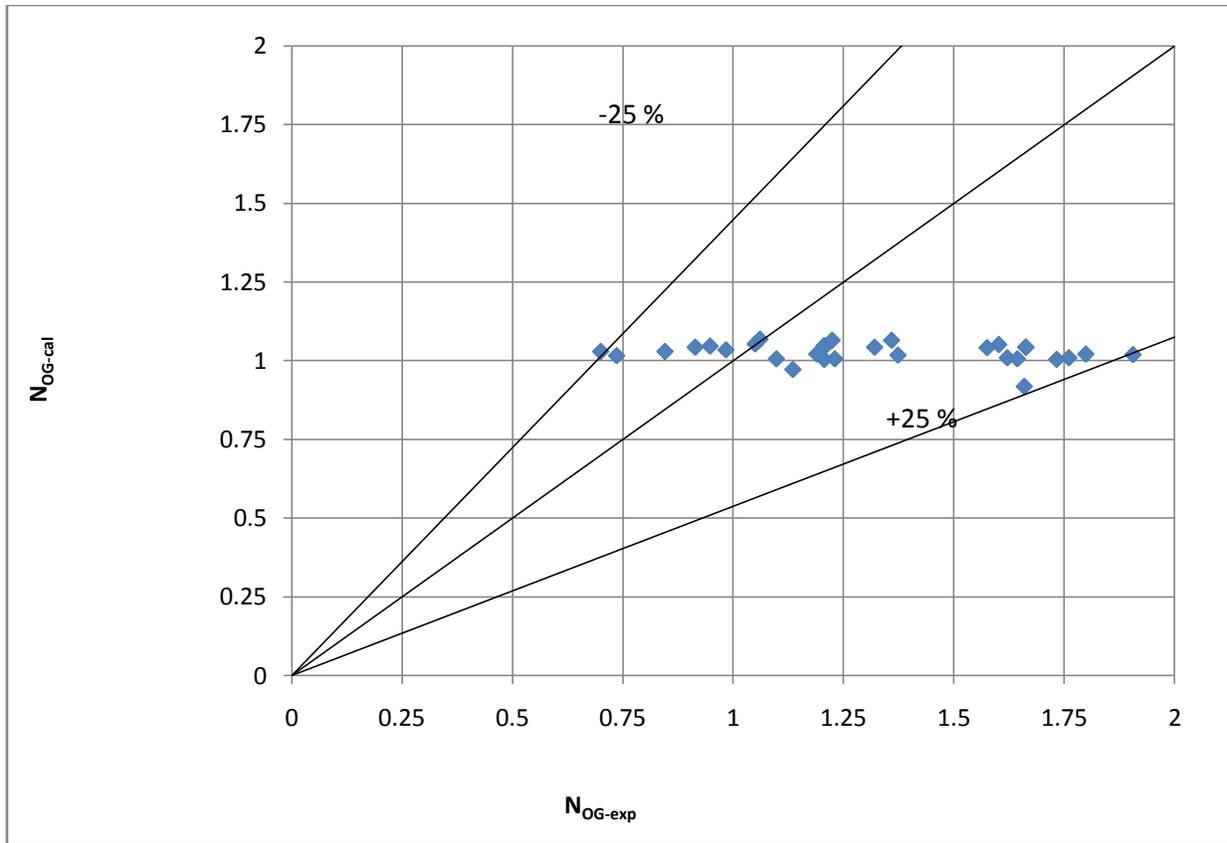


Fig. 6:- Comparison between the experimental data on the total number of mass-transfer units for the Tetrachloromethane-Toluene mixture and those calculated by the model

It can be seen from the comparison made in Fig. 5 that the applied model also enables the prediction of the total number of vapour phase mass-transfer units with a maximum error below $\mp 25\%$ compared to those obtained experimentally for the Tetrachloromethane-Toluene mixture.

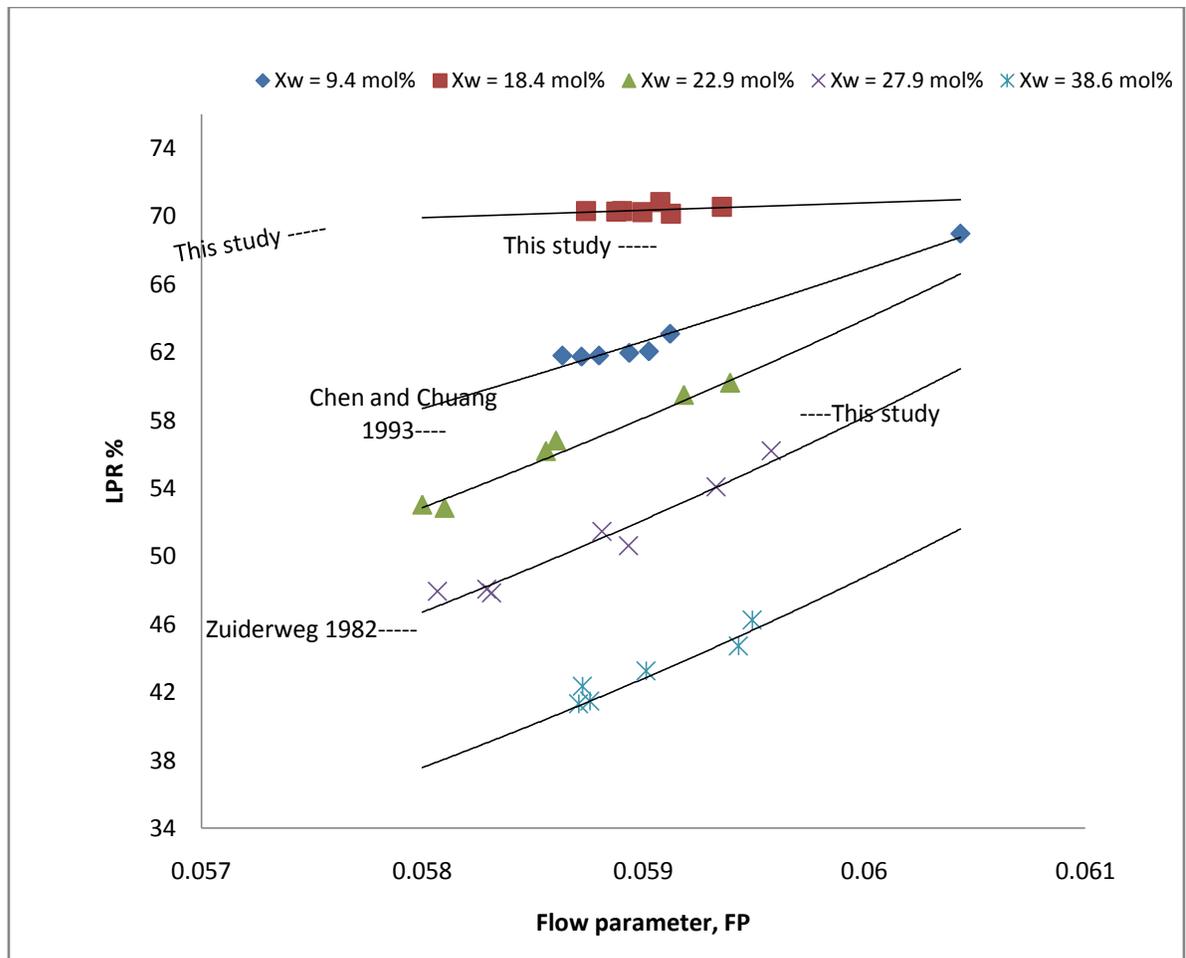


Fig. 7:- Comparison of the liquid phase resistance on the total resistance of the-mass transfer process, LPR%, for the Tetrachloromethane-Toluene mixture with LPR% of other models.

Porter and Jenkins (1979) 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 number of mass-transfer units, the local efficiency, the resistance that the liquid phase has on the total resistance of the mass transfer process and to predict them by existing models.

Fig. 7 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 (1982) and, at a concentration of HVC in the initial mixture of 22.9%, with those presented by applying Chen and Chuang's model (1993).

The match of the LPR% values obtained by the applied model with those presented by Zuiderweg (1982) and Chen and Chuang (1993) 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 (1993) gives high LPR% values compared to other models. For the studied mixture, higher LPR% values were obtained compared to Chen and Chuang's model (1993) 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. 7).

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 and the total number of mass-transfer units for the Tetra-chloromethane-Toluene model mixture was checked. The values of the constants in the model were determined ($C_1 = 11$ and $C_2 = 14$), using 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 $\pm 25\%$.

In a narrow load factor range $F_s = 0.17 \div 0.18 \text{ kg}^{0.5}/(\text{m}^{0.5} \cdot \text{s})$ for HVC concentrations in the initial mixture of 27.9% and 38.6% a match of the values of the local efficiency calculated by the model was found. For the studied mixture in the range of variation of the flow parameters FP from 0.0576 to 0.0604, corresponding to low vapour velocities, there was an increase in the number of vapour phase mass-transfer units calculated by the model.

With the increase of the concentration of HVC in the initial mixture from 9.4% to 38.6% and changing the flow parameters in the range $FP = 0.059 \div 0.0605$ corresponding to a vapour velocity $W_V = 0.0692 \div 0.088 \text{ m/s}$, a linear increase of the vapour phase local efficiency calculated by the model was recorded, the maximum error being below $\mp 25\%$.

A match of the LPR% obtained by the model was found: with the percentage given when applying Zuiderweg's model (1982) at an HVC concentration in the initial mixture of 38.6%, and with the percentage presented when applying Chen and Chuang's model (1993) at an HVC concentration in the initial mixture of 22.9%. Higher LPR% values were obtained compared to Chen and Chuang's model (1993) 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%.

The proposed model can be used to predict the local efficiency and the number of mass-transfer units in the rectification of any binary mixture depending on its physicochemical properties even at low vapour velocities.

Nomenclature

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

$K_{OG}, a, k_G, a, k_L, a$ - overall volume mass-transfer coefficient, vapour phase volume mass-transfer coefficient, liquid phase volume mass-transfer coefficient, $\text{kmol}/\text{m}^3 \cdot \text{s}$;

$\lambda = \frac{m \cdot G}{L}$ - diffusion potential;

m - slope of vapour-liquid equilibrium line;

G and L - vapour and liquid flow rate, kmol/s ;

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

a - interfacial area per unit volume of two-phase dispersion m^2/m^3 ; $a = \frac{1}{\mu^{0.1} \cdot \phi^{0.14}} \cdot \left[\frac{F_s^2 \cdot \rho_L}{\sigma^2} \right]^{1/3} \text{m}^2/\text{m}^3$;

t_G, t_L - holdup time of vapour 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 vapour volume spends on the interfacial area, s ;

h_L - clear liquid height on a sieve tray, $[\text{m}]$: $h_L = 0,6 \cdot h_w^{0.5} \cdot p^{0.25} \cdot \left[\frac{(\rho_G/\rho_L)^{0.5}}{b} \right]^{0.25}$;

LPR% - the percentage 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 - vapour and liquid phase densities, kg/m^3 ;

b - length of overflow threshold per unit working (bubbling) area of the tray, m ;

W_V - vapour velocity relative to the working area of the tray, m/s

F_s - load factor, $F_s = \text{superficial F-factor } F_s = W_V \cdot (\rho_G)^{0.5}, \text{ kg}^{0.5}/(\text{m}^{0.5} \cdot \text{s})$;

ϕ - fractional perforated tray area;

σ – surface tension, N/m²;

A and B – variables calculated using equations (14) and (15), respectively;

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

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14. Mariana KrustevaKaraivanova, PhD, Chief Assistant Professor, Chemical Technologies Department, Technical Sciences Faculty, Prof. Dr Assen Zlatarov University, 1 Prof. Yakimov Blvd, Burgas, E-mail:anamariana@abv.bg,
15. DesislavaRadkovaKoleva, PhD, Chief Assistant Professor, Chemical Technologies Department, Technical Sciences Faculty, Prof. Dr Assen Zlatarov University, 1 Prof. Yakimov Blvd, Burgas,E-mail:desikol@abv.bg.