RESEARCH ARTICLE

STUDY OF INTERFACIAL AREA IN RECTIFICATION OF TWO-COMPONENT MIXTURES

Mariana Karaivanova

Manuscript Info	*Abstract*
	One of the main problems with tray rectification apparatuses is the kinetic studies of mass exchange, which are complicated due to difficulties in determining the volumetric interfacial area formed during the dispersion of the vapour phase in the liquid on the tray as well as the mixing of the liquid as it moves on the tray and the presence of impurities in the separated mixtures. The interfacial area is a major characteristic of the gas-liquid layer on the tray and directly affects the mass-transfer process. The present work aims to contribute to this area of study by proposing an experimental computational method for determining the volumetric interfacial area, α. The method is only applicable for the studied laboratory single-sieve tray glass column.

Introduction:-

Mass exchange processes are among the most common and most important processes in the chemical industry. They involve the transfer of one or more substances from one phase to another. These processes are used for the separation of heterogeneous and homogeneous gas and liquid mixtures into simple components or fractions. This group of processes features the processes for fluid-fluid separation, namely adsorption, distillation, rectification and extraction.

In a number of cases, the efficiency of an apparatus in which a mass exchange process takes place has to be evaluated using both the mass transfer coefficient (the amount of substance transferred per time through an interfacial surface area at a driving force) and the efficiency coefficient.

One of the main problems with tray rectification apparatuses is the kinetic studies of mass exchange, which are complicated due to difficulties in determining the volumetric interfacial area formed during the dispersion of the vapour phase in the liquid on the tray as well as the mixing of the liquid as it moves on the tray and the presence of impurities in the separated mixtures [1].

The interfacial area is a major characteristic of the gas-liquid layer on the tray as it directly affects the mass-transfer process. To calculate the interfacial area, a number of empirical correlations attained after summarizing experimental data obtained via different methods (photographic, chemical) mainly for sieve trays have been proposed [2-4]. These correlations have limited validity for the studied tray design.

It should be noted that most studies aimed at determining the interfacial area are experimental. This is due to the lack of universal analytical or mathematical methods for the calculation of the interfacial area for separation and

---

Corresponding Author:- Mariana Karaivanova

heat transfer processes which could be used to more easily develop innovative separation equipment and solve the problem of optimum layout in the initial design stage.

The aim of the present work is to propose an analytical solution for the determination of the interfacial area in the separation by rectification of the following binary mixtures: Water – Acetic acid, Tetrachloromethane – Toluene and Dichloroethane – n-Propyl alcohol under conditions of complete mixing of the liquid phase and mode of ideal displacement by vapour phase. To approximate these ideal motion patterns of the two phases the experiments were carried out in a small-scale single-sieve laboratory glass column [5].

Computational
In mass exchange processes, the two phases between which the transfer of a substance takes place come into direct contact with each other. As a result, during the process the so-called interfacial area is formed.

A typical feature of the interfacial area in bubble cap columns is its flexible (dynamic) character. The interfacial area depends on the hydrodynamic modes, which in turn depend on the flow rates of the two fluids and the design of the contact device [6].

The calculation of the volumetric interfacial area in rectification for the three mixtures studied is based on a proposed method which applies a comparison between the experimentally obtained total volumetric coefficient of vapour phase mass transfer $(K_{OG}.a)^{exp}$ and the total vapour phase mass transfer coefficient calculated using Higbie's penetration model for the same mixtures and conditions $(K_{OG})^{cal}$[7].

$$\alpha = \frac{(K_{OG}.a)^{exp}}{(K_{OG})^{cal}} \qquad (1)$$

The method has an experimental computational character, because α, [m ^{2}/m^3] is determined by processing both experimental and theoretically calculated data. The method is applicable only for the studied laboratory model column with a single sieve tray when the following conditions are observed:
- the liquid phase moves in a full mixing mode on the tray;
- the vapour phase moves in a full displacement mode (piston mode);
- the column operates in a full reflux mode at atmospheric pressure;
- a model sieve tray with external outlet weirs is installed in the column.

The calculation of the total mass transfer coefficient of the vapour phase is based on the additivity principle of phase resistances, the penetration model and Higbie's model [8, 9]:

$$\frac{1}{(K_{OG})^{cal}} = \frac{1}{\beta_G} + \frac{m}{\beta_L} \qquad (2)$$

According to the additivity principle of phase resistances, the total resistance of the process is the sum of the resistances in the individual phases.

According to the penetration model, to describe the transfer of a substance through a mobile interfacial area, it is assumed that turbulent eddies carry certain volumes of fluid from the flow core to the edge area. For the short contact time, the molecules of the diffusing substance are transferred to the other phase through nonstationary diffusion, also known as penetration. The reacted elements are then taken back to the core of the stream and new ones are brought in in their place.

According to Higbie's model, the mass transfer coefficients for the vapour and liquid phases at equal contact time for all elements are calculated using the following dependence [8]:

$$\beta_G = \sqrt{\frac{4.D_G}{\pi.\theta_G}} \qquad (3)$$

$$\beta_L = \sqrt{\frac{4.D_L}{\pi.\theta_L}} \qquad (4)$$

The calculation of the molecular diffusion coefficient for the vapour phase D_G and the liquid phase D_L is carried out by means of the following formulae [2, 10]:

$$D_G = \frac{4.3.10^{-7}.T^{3/2}}{p.\left(\vartheta_A^{1/3}+\vartheta_B^{1/3}\right)^2} \cdot \sqrt{\frac{1}{M_A}+\frac{1}{M_B}} \qquad (5)$$

$$D_L = \frac{K.M_B^{1/2}.T}{\mu_B.(V_A.V_B)^{1/3}} \qquad (6)$$

We assume that the contact time for the vapour phase is equal to the residence time of the vapour phase in the gas-liquid layer, i.e. the following dependence is in force:

$$\theta_G = \frac{h_L}{w_n} \qquad (7)$$

The contact time for the liquid phase θ_L is calculated by means of the dependence:

$$\theta_L = \theta_G.\frac{\rho_G}{\rho_L} \qquad (8)$$

To determine the total volumetric mass transfer coefficient by vapour phase $(K_{OG}.a)^{exp}$ the following equation is used:

$$(K_{OG}.a)^{exp} = \frac{w_n.\rho_G.[-\ln(1-E_{OG})]}{h_n.M_G} \qquad (9)$$

The volumetric interfacial area is calculated using the following equation, where h_n and E_{OG} are determined experimentally and $(K_{OG})^{cal}$ is calculated using the methodology proposed above. This determines the experimental computational nature of the present method for calculating the volumetric interfacial area α, m²/m³.

$$\alpha = \frac{w_n.[-\ln(1-E_{OG})]}{h_n.(K_{OG})^{cal}} \qquad (10)$$

The relative deviation in the determination of the volumetric interfacial area is calculated by the following equation:

$$\Delta = \frac{a_{cp}-a}{a_{cp}}.100, \ \% \qquad (11)$$

The standard deviation S_a is calculated using formula (11):

$$S_a = \sqrt{S_{ai}^2} \qquad (12)$$

The dispersion S_{ai}^2 of the values calculated by means of the developed methodology for the volumetric interfacial area is calculated by the formula:

$$S_{ai}^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(a_i - a_{cp}\right)^2 \qquad (13)$$

Results and Discussion:-

The effect of the column vapour velocity w_n on the calculated values of the relative interfacial area α determined by the proposed methodology for the three binary mixtures Water – Acetic acid, Tetrachloromethane – Toluene and Dichloroethane – n-Propyl alcohol is presented in Fig. 1:
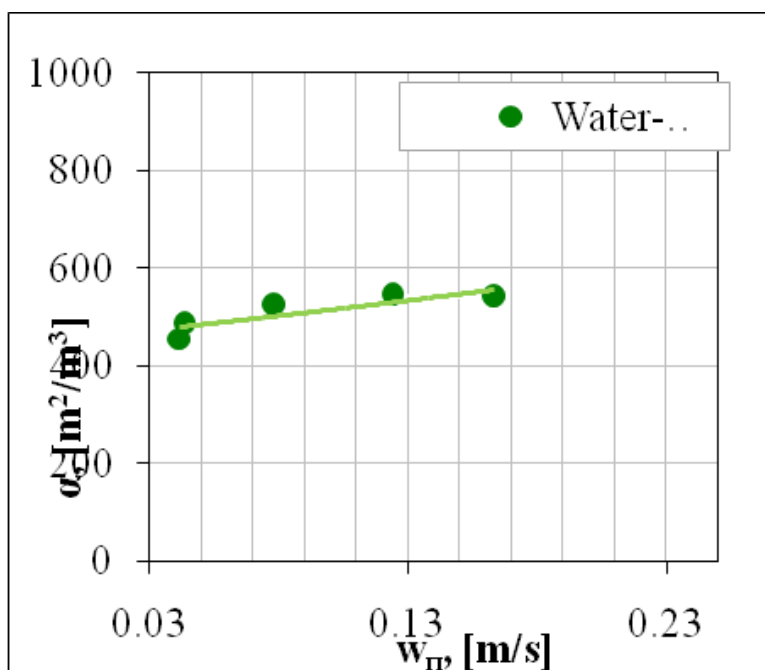
Fig. 1:- Dependence of the relative interfacial area α on the vapour velocity w_n in the column determined by the proposed methodology for the Water – Acetic acid binary mixture

As can be seen from Fig. 1, the increase of the vapour velocity (about 4 times) led to a minor increase of the relative interfacial area of the Water – Acetic acid mixture for the whole velocity interval studied (about 15%).

For the Tetrachloromethane – Toluene binary mixture, the increase of the vapour velocity in the column from 0.029 to 0.081 m/s led to a significant decrease of the relative interfacial area for the whole velocity interval studied (about 35%) (Fig. 2):
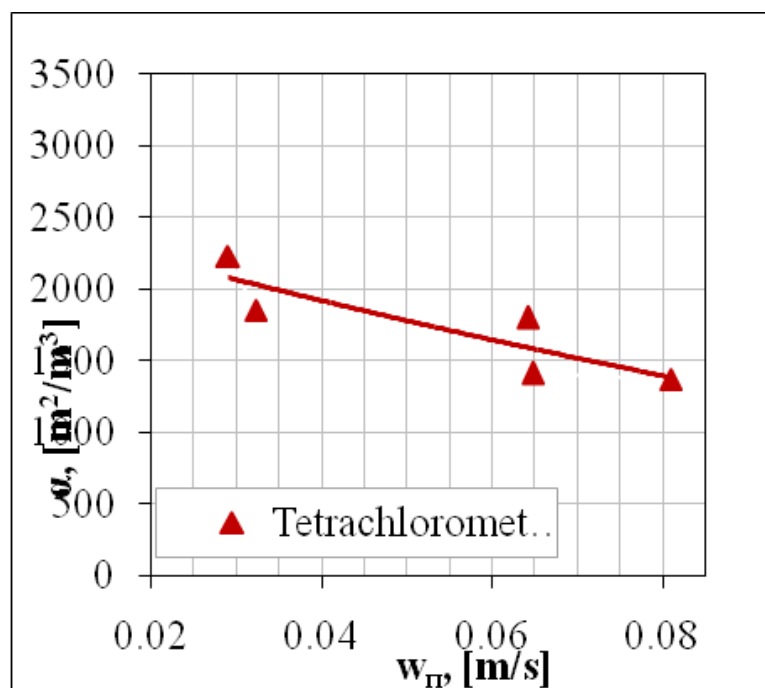

Fig. 2:- Dependence of the relative interfacial area α on the vapour velocity w_n in the column determined by the proposed methodology for the Tetrachloromethane – Toluene binary mixture.
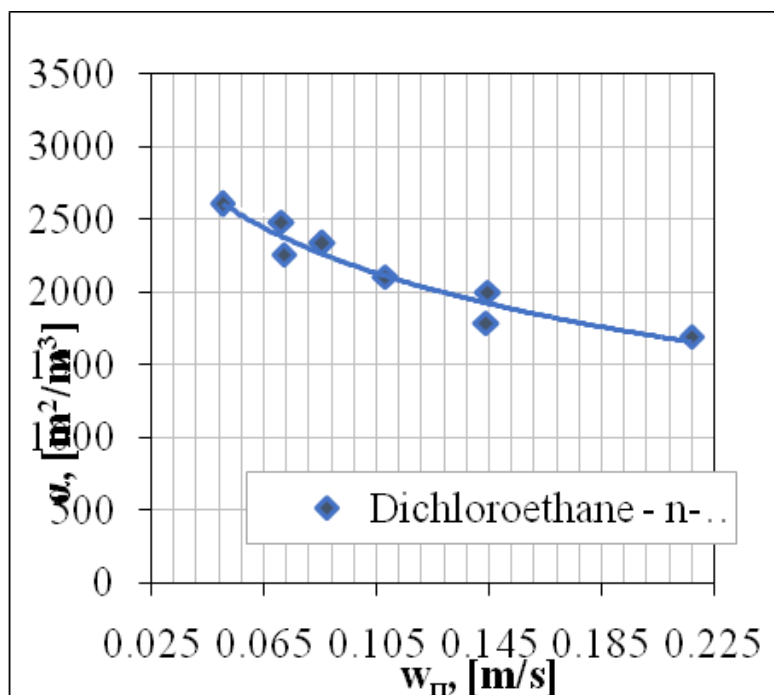
Fig. 3:- Dependence of the relative interfacial area α on the vapour velocity w_π in the column determined by the proposed methodology for the Dichloroethane – n-Propyl alcohol binary mixture.

As can be seen from Fig. 3, for the Dichloroethane – n-Propyl alcohol binary mixture the increase of the vapour velocity from 0.05 to 0.22 m/s led to a decrease of the relative interfacial area by about 35%.

Fig. 4 presents the dependence of the relative volumetric interfacial area calculated by the proposed methodology on the separation efficiency (local efficiency) of rectification for the three model mixtures. In all three model mixtures studied, the greater separation efficiency corresponds to larger values of the relative interfacial area, which is logical and could be a precondition for a quantitative relationship between the interfacial area formed in the gas-liquid layer of sieve tray columns and the separation efficiency of rectification.
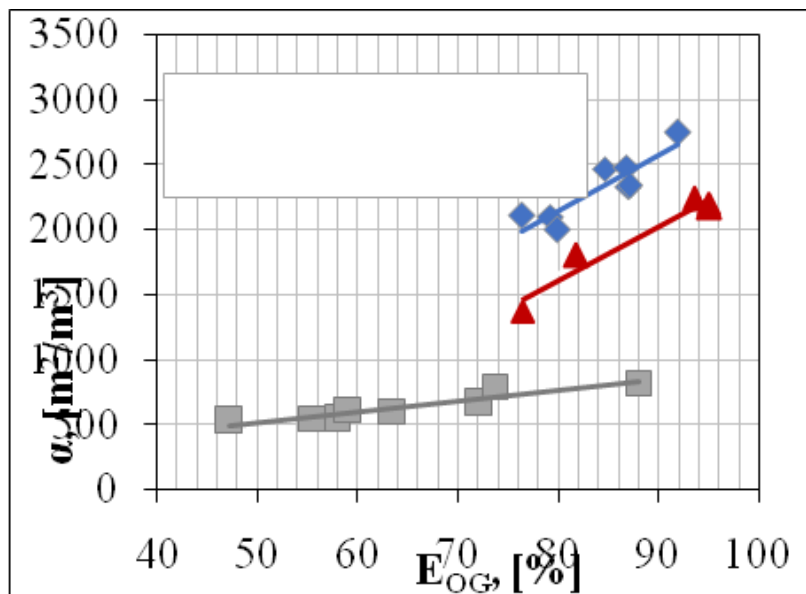

Fig. 4:- Dependence of the relative interfacial area α on the local efficiency E_{OG} for the three binary mixtures: Water – Acetic acid, Tetrachloromethane – Toluene and Dichloroethane – n-Propyl alcohol

Conclusions:-

1. By means of the proposed methodology, the values of the volumetric interfacial area "α" for three binary mixtures, Water – Acetic acid, Tetrachloromethane – Toluene and Dichloroethane – n-Propyl alcohol, have been determined on the basis of experimental data obtained by rectification in a single-sieve tray laboratory column. As a result of the calculations, the relative error in determining the volumetric interfacial area is about 14% for the Water – Acetic acid and Tetrachloromethane – Toluene mixtures and 10% for the Dichloroethane – n-Propyl alcohol mixture.
2. It has been established that the relative volumetric interfacial area for the Water – Acetic acid binary mixture increases slightly with the increase of the vapour velocity in the column. For the investigated velocity interval from 0.042 to 0.16 m/s, the decrease was approximately 15%.
3. For the Tetrachloromethane – Toluene binary mixture, the effect of the vapour velocity in the column on the value of the volumetric relative interfacial area is also significant, but decreases about twice.
4. For the Dichloroethane – n-Propyl alcohol binary mixture, the increase of vapour velocity from 0.05 to 0.22 m/s results in a decrease of the relative interfacial area by about 1.5 times.
5. In all three mixtures studied, the higher values of the relative volumetric interfacial area result in higher values of the local efficiency of the process (more significantly for the Tetrachloromethane – Toluene and Dichloroethane – n-Propyl alcohol mixtures).
6. The resulting standard deviation S_α of the values of the volumetric interfacial area calculated by the proposed methodology (251 m^2/m^3 for Water – Acetic acid, 714 m^2/m^3 for Tetrachloromethane – Toluene and 676 m^2/m^3 for Dichloroethane – n-Propyl alcohol) from the average values obtained for the three binary mixtures (643.35 m^2/m^3 for Water – Acetic acid, 1846.69 m^2/m^3 for Tetrachloromethane – Toluene and 2274.3 m^2/m^3 for Dichloroethane – n-Propyl alcohol) shows that the magnitude of the interfacial area is significantly affected both by the hydrodynamics of the process and the initial concentration of the separated mixture.

Nomenclature

a - specific interfacial area, [m^2/m^3]
D_G – molecular diffusion coefficient of the vapour phase, [m^2/s]
D_L – molecular diffusion coefficient of the liquid phase, [m^2/s]
E_{OG} – efficiency coefficient of the tray, local efficiency, %
$h_п$ - height of an ellipsoidal bubble, [m]
h_L – height of the light liquid, [m]
$K_{OG}.a$ - overall mass transfer coefficient, [$kmol/m^3.s$]
K_{OG} - gas-side mass transfer coefficient, [$m.s^{-1}$]
M - molecular weight, [kg/kmol]
P – absolute pressure, [Pa]
$w_п$ – vapor velocity, [m/s]
$β_G$ - vapour-phase mass transfer unit, [m/s]
$β_L$ - liquid-phase mass transfer unit, [m/s]
$ρ_G$ - gas density, [kg/m^3]
$ρ_L$ - liquid density, [kg/m^3]
$μ_G$ - gas viscosity, [Pa.s]
$μ_L$ - liquid viscosity, [Pa.s]

References:-

1. Tasev, Zh., On some basic chemical engineering problems in the creation of highly efficient rectification apparatuses, Doctoral thesis, HIChT-Burgas, **1997.**
2. Hofer, H., A. Mersmann, Chem. Ing. Techn., 52, 248, **1982.**
3. Kaufmann K. D., T. Pilofer, Chem. Ing. Techn., 52, 248, **1982.**
4. Stefanov, Zh., Zh. Tasev, Annual of VHTI, Burgas, vol. 16, 1, 165, **1981**.
5. Ivanov, Zh., Zh. Stefanov, Zh. Tasev, Total volumetric mass transfer coefficient in rectification of binary mixtures, Annual of Prof. Dr Assen Zlatarov University, Burgas, vol. 35, book 1, 43-46, **2006**.
6. Akita, K., F. Yoshida, Ind. Eng. Chem. Process, Des, Dev, 12, 84, **1974.**
7. Stefanov, Zh., Zh. Ivanov, D. Radev, Comparison between two different models to predict interfacial mass transfer area in distillation column with sieve tray, Science & Technologies, Vol. 2, 4, 31-36, **2012.**

8. Higbie, R., The rate of absorption of a pure gas into a still liquid during short periods of exposure, Transactions of the I.I.Ch.E., 31, 365-389, **1935**.
9. Chen G. X., K. T. Chuang, Prediction of point efficiency for sieve tray in distillation, Industrial and Engineering Chemistry Research, 32, 4, 701-708, **1993**.
10. Tasev, Zh., D. Mitev, R. Kutsarov, Zh. Stefanov, D, Varbanov, H. Genchev, V. Rashev, Course guide on the design of processes and apparatuses in the chemical industry, **1986.**
11. Kamenski, D., Experimental research and optimization methods, VHTI Publishing, Burgas, **1990.**