Abstract—Using plug flow model in conjunction with experimental solute concentration profiles, overall volumetric mass transfer coefficient based on continuous phase ($K_{oa}$), in a packed liquid-liquid extraction column has been optimized. Number of 12 experiments has been done using standard system of water/acidic acetic/toluene in a 6 cm diameter, 120 cm height column. Thorough consideration of influencing parameters we intended to correlate dimensionless parameters in term of overall Sherwood number which has an acceptable average error of about 15.8%.

Keywords—Packed column, mass transfer coefficient, solvent extraction, Sherwood number.

I. INTRODUCTION

Packed liquid-liquid extraction columns are widely employed in industrial practice. The flow of liquids in the column is brought out by the difference in densities of the two liquid phases. Either liquid may be made continuous or dispersed by the use of suitable distributors and the position of the liquid-liquid interface. The presence of packings in the column increases the local velocities, retards recirculation and back-mixing and improves the distribution and hold-up of the dispersed phase. Wiegandt and Von Berg [1] have shown that the height of a packed column required to affect a given degree of extraction is reduced by a factor of three, under pulsing conditions. Overall volumetric mass transfer coefficient ($K_{oa}$) is one of the most important parameters required for design and scale up of an extraction column. Estimation of this parameter however is just attainable using experimental solute concentration profiles in conjunction with mathematical mass transfer models such as plug flow, axial dispersion, backflow or forward mixing. Within these models, ideal plug flow model is the simplest one, has a widespread use in industrial and scale up design [2,3]. For a better scale up it is conventional to present affecting parameters in a dimensionless form hence mass transfer coefficient usually come along with Sherwood number. In this work by describing plug flow model in a simplified dimensionless style, overall volumetric mass transfer coefficient will be calculated by optimizing the model with experimental concentration profiles. A new correlation for Sherwood number will be developed in which effect of operational variables have been considered.

II. MASS TRANSFER MODELING BASED ON PLUG FLOW ASSUMPTION

Plug flow is the simplest possible modeling in which we assume that in each phase all elements have just one residence time in the column [2]. In other words all parts of for example continuous phase elements past the column in equal time periods ($t=HS/Q_c$). As shown in Fig 1 applying plug flow model, solute mass balance in a control volume of height of $dz$ for each phase has three terms.

$$Q_c \rho \frac{dx}{dz} - Q_c \rho \frac{x_L}{L} - K_{oa}(x-x^*)S(1-\phi)dz = 0 \quad (1)$$

$$Q_d \rho \frac{y}{L} - Q_d \rho \frac{y_L}{L} + K_{oa}(x-x^*)S(1-\phi)dz = 0 \quad (2)$$

Fig. 1 Schematic view of solute mass balance in height of $dz$ of an extraction column based on plug flow model

The last terms in (1) and (2) represent the mass transferring from interface of phases. Rearrangement and normalizing of (1) and (2).

$$- \frac{dX}{dZ} + NTU_{ac} (X + Y - 1) = 0 \quad (3)$$

$$- \frac{dY}{dZ} - \frac{NTU_{ac}}{\Omega} (X + Y - 1) = 0 \quad (4)$$

Equations (3) and (4) are a set of first order ODEs and we need one boundary condition for each to be solved.
analytically. Usually the entrance concentration of phases are known, so the boundary conditions are \( X(0) = 0 \) and \( Y(0) = 0 \). Using operator procedure to solve differential equations of (3) and (4):

\[
X(Z) = \frac{\Omega(\exp(\Gamma Z) - \exp(\Gamma))}{1 - \Omega \exp(\Gamma)} \\
Y(Z) = \frac{1 - \exp(\Gamma Z)}{1 - \Omega \exp(\Gamma)}
\]

III. EXPERIMENT

Fig. 2 shows a schematic view of a packed extraction column. Our column is a pilot, 6 cm diameter with a packed section height of 1.2 m. Packings are stainless steel rasching rings which provide a porosity of about 0.74. Operating conditions of runs are listed in Table I. Number of 12 experiments was done with water/acetic acid/Toluene standard system which is known as a system with high interfacial tension. In all experiments, acetic acid is solute, water is continuous phase and Toluene is the dispersed phase and mass transfer direction is from dispersed to continuous phase. Applying Titration concentration analysis, solute concentration profiles in column vertical axes will be determined.

IV. RESULT AND DISCUSSION

Although it isn’t ever done in mass transfer literatures to assess an overall Sherwood number but in almost all published correlations of individual phase Sherwood (Sh_d and Sh_c), the resistance against mass transfer in the other phase has been ignored which will make large errors. So we were persuaded to correlate affecting parameters in term of an overall Sherwood number.

\[
Sh_{oc} = 0.0069 \left( \frac{Re^{1.12}}{(\phi(1-\phi))^0.5} \left( \frac{U_c}{U_d} \right) \right)^{1.01}
\]

In which \( Sh_{oc} = K_{oc}d_{32}/D_z \) is the overall Sherwood number and \( Re = U_c d_{32} \rho_c/\mu_c \) is the drop Reynolds number. The last column in Table I shows deviation of Eq. (7) from experimental results. The net average error is about 15.7% which is practically acceptable. Experimental Sherwood and model is shown in Fig. 3.

<table>
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<tr>
<th>Run no.</th>
<th>Qc (ml/min)</th>
<th>Qd (ml/min)</th>
<th>d_{32} (mm)</th>
<th>Dispersed phase hold up (%)</th>
<th>Re</th>
<th>Percent error of Eq.(7)</th>
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Fig. 2 Schematic view of a packed extraction column.

Fig. 3 Comparison between experimental Sherwood and model.

TABLE I

OPERATING CONDITIONS AND PERCENT ERROR OF EQUATION (7) FOR EACH RUN

Fig. 2 Schematic view of a packed extraction column.
**SYMBOLS**

**English symbols**
- Interfacial area per unit volume (m²/m³): \( a \)
- Solute diffusion coefficient: \( D \)
- Sauter mean drop diameter: \( d_{32} \)
- Pulse frequency (1/s): \( f \)
- Continuous phase concentration (%wt): \( x \)
- Dispersed phase concentration (%wt): \( y \)
- Axial dimension (height) of column (m): \( z \)
- Column height (m): \( H \)
- Volumetric phase flow (m³/s): \( Q \)
- Velocity: \( U \)
- Column cross section (m²): \( S \)
- Overall mass transfer coefficient (m/s): \( K \)

**Greek symbols**
- Phase Density (Kg/m³): \( \rho \)
- Phase viscosity (Kg/m.s): \( \mu \)
- Porosity of packing: \( \epsilon \)
- Dispersed phase hold up: \( \phi \)

\[ \text{Number of Transfer Unit (NTU): } NTU_{oc} = \frac{HS}{1 - \phi} \frac{K_{oc} a}{Q_c} \]

\[ \Gamma = \frac{m Q_d \rho_d}{Q_c \rho_c} \]

\[ \Omega = \left( 1 - \frac{1}{\Omega} \right) NTU_{oc} \]

**subscripts**
- Dispersed phase: \( d \)
- Continuous phase: \( c \)
- Overall based on (c or d): \( o \)
- Inlet to column: \( in \)
- Outlet from column: \( out \)
- Slip: \( s \)

**Superscript**
- Equilibrium state: \( \ast \)

**Dimensionless symbols**
- Distribution coefficient: \( y = m x^* \)
- \( \left( x - x_{in} \right) \left( x_{oc}^* - x_{in}^* \right) \)
- \( \left( y - y_{in} \right) \left( y_{oc}^* - y_{in}^* \right) \)

**REFERENCES**