

## Prediction of Efficiency and Solute Concentration along RDC Column with Applying New Effective Diffusivity Correlation

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**Abstract:** Liquid-liquid extraction is one of the most important separation processes. Different kinds of liquid-liquid contactors such as RDC, Pulsed columns ... are being used in industries. Determination of solute concentration and mass transfer coefficients as one of the fundamental parameters is of great importance in RDC column design. This research is devoted to calculating efficiency and solute concentration along column with the use of existing correlations and new proposed effective diffusivity correlation. Finally the results will be juxtaposed with experimental values for the aforesaid parameters. Prediction of concentration variation along the column will result in more accurate prediction of physical properties variations along the column, which can be used for designing of columns by researchers. The results indicated that the new effective diffusivity include slightest error for predicting efficiency and solute concentration. Accordingly, use of these equations lead in a more accurate design scheme.

**Key words:** Liquid-liquid extraction, RDC column, Efficiency, Concentration variation

### INTRODUCTION

RDC columns are one of the most important extract columns, which have extensive application in various industries. During column design different parameters will be studied, such as dispersed phase and continues phase mass transfer coefficients that have importance during RDC column design and a lot of correlations existing for them (Newman, 1931; Johnson and Hamielec, 1960; Lochiel and Calderbank, 1964; Steiner, 1986; Temos *et al.*, 1993). With employ of these correlations, mass transfer coefficient, column efficiency and solute concentration variation along column can be predicted.

In next sections with use of several presented correlations, and also with use of presented correlation with authors of this paper for calculating of effective diffusion (Bahmanyar *et al.*, 2009), efficiency and solute concentration at different points of column have been calculated. These values have been compared with experimental values at every stages and error percentage have been calculated.

Physical properties variation can be predicted along the column with apply of solute concentration prediction at different distance of column.

#### Previous work:

With regard to the drop size and behavior for clean systems, the mass transfer mechanism and mass transfer coefficients will be varied in the RDC. One of the oldest of these equations which is used for stagnant drops with molecular diffusion mechanism is the Newman equation (Newman, 1931), which will result in equation (2) by using the continuity equation and applying the initial and boundary conditions as follows:

$$\frac{\partial C}{\partial t} = D_d \left[ \frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right] \quad (1)$$

I.C:  $C(r,0)=C_0$

B.C<sub>1</sub>:  $C(r_s,t)=C^*$

B.C<sub>2</sub>  $\lim C(r,t)=\text{bounded}$

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While  $r \rightarrow 0$

Where  $r_s$  is the drop radius.

Thus the Newman equation can be written as:

$$E = \frac{C_s - C^*}{C_0 - C^*} = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \left[ \frac{1}{n^2} \exp(-4n^2 \pi^2 D_d t / d^2) \right] \quad (2)$$

Considering the mass balance for droplet we get:

$$K_d = \frac{-d}{6t} Ln[1 - E] \quad (3)$$

If the continuous phase resistance exists, combination of Eqs. (2) and (3) will be:

$$K_d = \frac{-d}{6t} Ln \left[ \frac{6}{\pi^2} \sum_{n=1}^{\infty} C_n \exp(-4 \lambda_n^2 D_d t / d^2) \right] \quad (4)$$

Where  $C_n$  and  $\lambda_n$  are functions of  $K_d d / D_d$ . (Elzinga and Banchemo, 1959).

In the future, in order to more accurately calculate the mass transfer coefficient, researchers have replaced the diffusion coefficient with the effective diffusion coefficient or enhancement factor, which includes all the effective elements on these coefficients in the Newman equation.

Many equations have been presented for determining the enhancement factor of which several have been pointed out below:

1-Johnson and Hamielec (1960):

$$R = dU_t / 2048(1 + k)D_d \quad (5)$$

2 -Lochiel and Calderbank (1964):

$$R = 1 + [dU_t / 2048(1 + k)D_d] \left\{ 1 - \left[ \frac{(2 + 3k)}{1 + (\mu_d \rho_d / \mu_c \rho_c)^{0.5}} \right] \frac{1.45}{Re^{0.5}} \right\} \quad (6)$$

3-Davis (1966):

$$R = \frac{D_{oE}}{D_d} = f_v + (1 - f_v) \left[ \frac{k_H U_t d}{2048(1 + k)D_d} \right] \quad (7)$$

$$f_v = 1 - \exp[-(0.098Eo / k)^{-2.21}] \quad (8)$$

$$Eo = g d^3 \Delta \rho / \gamma \quad (9)$$

$$E_{oc} = 6k \quad (10)$$

4-Boyodzhiev *et al.*, (1969):

$$R = 0.003(\rho_d d U_t / \mu_c)^2 [1/(1 + k)]^2 \quad (11)$$

5-Steiner (1986):

$$R = 1 + 0.177 Re^{0.43} Sc_d^{0.23} [1/(1 + k)]^{0.80} \quad (12)$$

6-Temos *et al.*, (1993):

$$D_{oE} = D_d + 0.44 D_E \quad (13)$$

$$\rho_d D_E / \mu_d = 3.29 \times 10^{-4} (\rho_d d U_i / \mu_d) [1 - \exp(3.29 \times 10^{-4} \rho_d d U_i / \mu_d)] \quad \text{for } Re \ll 1$$

$$U_i = \left\{ 1 - \left[ \frac{(2 + 3k)}{1 + (\mu_d \rho_d / \mu_c \rho_c)^{0.5}} \right] \frac{1.45}{Re^{0.5}} \right\} U$$

In addition to above equations, another correlation has been presented by authors of this paper for calculating effective diffusivity which have less errors related to existing correlations. Consequently use of this equation for calculating efficiency and solute concentration along RDC column and finally appropriate design of column will be proposed.

The correlation of Bahmanyar, Zarkeshan and Amanabadi (2009) is:

$$D_{eff} = 0.4755 \times 10^{-9} (Re^{0.6501}) \quad (14)$$

$$Re = (\rho U_s d_{32}) / \mu_c \quad (15)$$

Where,  $U_s$  is the slip velocity which can be calculated using equation (16);

$$U_s = \frac{Q_c}{A(1 - \epsilon)} + \frac{Q_d}{A\epsilon} \quad (16)$$

All of the above equations have been used in the experimental results section and the achieved experimental results and results obtained from the above equations have been compared.

**Experimental Set Up, Chemical Systems and Operating Conditions**

The RDC column used in this study is made of glass and its rotors and stators are made of stainless steel. By using the existing valves in different sections of the column, there will also be possibility for sampling. Other geometrics of the column are tabulated in table (1).

**Table 1:** RDC column characteristics

Column height (cm)	90
Inner diameter of column (cm)	7.0
Inner diameter of stator (cm)	6.0
Outer diameter of rotor (cm)	5.0
Compartment height (cm)	2.5
Number of compartments in active region	2.8

The chemical system used in this study is water/ acetic acid / carbon tetrachloride, in which water is the continuous phase, acetic acid as the solute and carbon tetrachloride as the dispersed phase. Mass transfer direction in this system is from dispersed to continuous phase. Physical properties of the system are shown in table 2.

**Table 2:** physical properties of system ( T=20 °C , P= 1 atm)

Physical properties	Water/acetic acid/carbon tetra chloride
$\rho_c$ (kg/m <sup>3</sup> )	1000
$\rho_d$ (kg/m <sup>3</sup> )	1590
$\mu_c$ (kg/m.s)	0.001
$\mu_d$ (kg/m.s)	0.00095
$\gamma$ (N/m)	0.045

In each experiment carried out rotating velocity, phases flow rate and initial solute concentration in feed flow and final concentration in solvent flow are specified using digital tachometer photo / contact type, rotometer and titration with soda respectively. Inlet solvent stream is also nearly pure.

The average diameter of drop is obtained by taking pictures from the column in a number of positions. Hold up is obtained by shut down method. Operation conditions and above mentioned parameters for this system have been tabulated in table-3.

**Table 3:** operating conditions

Run	N (rpm)	Qc (lit/hr)	Qd (lit/hr)	Xt (gr/lit)	y t (gr/lit)	d32 (mm)	holdup * 100
1	400	30	30	3.83	2.24	1.42	4.39
2	1300	30	30	37.1	35.6	0.78	16.12
3	700	50	50	23.56	16.34	1.07	8.93
4	700	75	75	22.15	16	1.07	12.56
5	972	33.33	66.66	20.3	39.5	0.9	15.53

**Calculation of Solute Concentration and Efficiency along the Column by Using of the Presented Equations in the past Literature and Proposed Equation in this Work:**

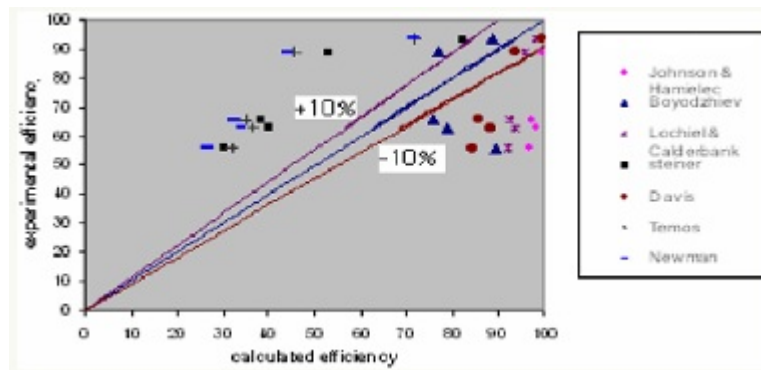
In this investigation, by using mentioned equations in the previous sections and substituting,  $t$ , ( $t=L/U_s$ , where  $L$  is height of the column at different position and  $U_s$  is droplet slip velocity) and also by using of presented correlations for correction factor ( $R$ ) efficiency and solute concentration in each stage along the column have been calculated.

**Efficiency:**

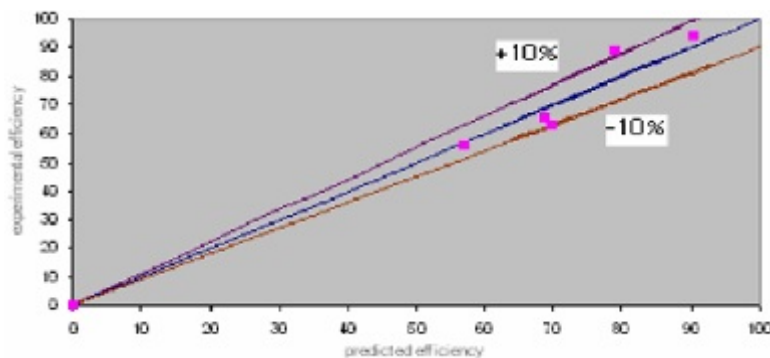
With using of existing relations and supposed  $D_{eff}$  relation respect to Reynolds number of droplet, efficiency along column has been calculated. Calculated efficiency from previous works and the proposed effective diffusivity equation have been compared with the experimental results in figures 1 and 2 and the absolute percentage of error is given in table-4 for all runs. According to this table among existing correlations, using of  $D_{eff}$  will results less error.

**Solute Concentration:**

Solute concentrations have been calculated along the column from pervious works. The results found from equation 14 (this work) and previous works are shown for run 1 in figures 3 and 4 and tabulated in table 5 for run 2 as an example. The average percentage of error found for other runs along the column (6 points for each run along the column) have been compared with the results of this work in table 6.



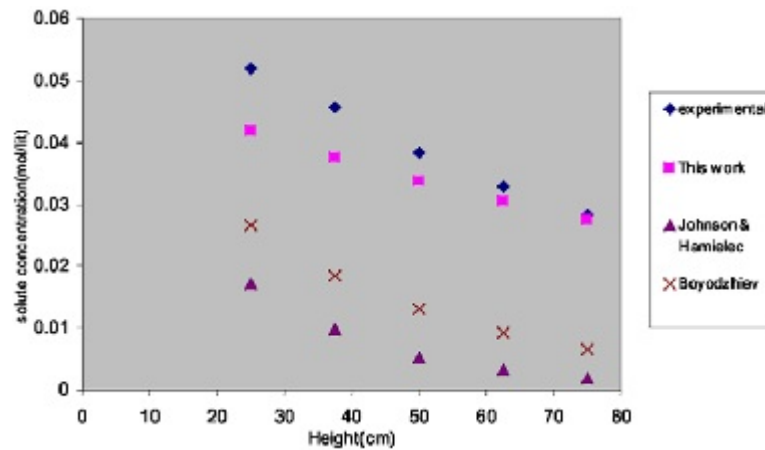
**Fig. 1:** Comparing of calculated efficiency using pervious correlations with experimental values



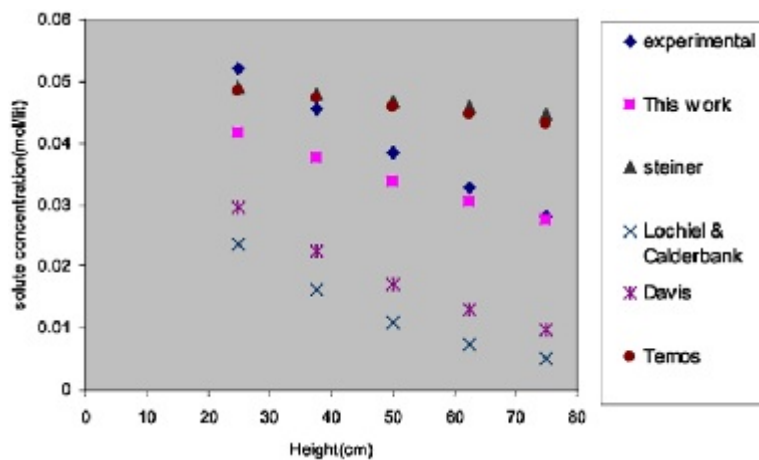
**Fig. 2:** Comparing of calculated efficiency with use of proposed correlation and experimental values

**Table 4:** Comparison of efficiency found from pervious works and experimental results

Previous work	Abs (% error)
Johnson & Hamielec	39.44
Boyodzhive	24.00
Steiner	35.53
Lochiel & Caldr banR	33.33
Davis	26.82
Temos	40.82
Newman	44.76
This work	6.43



**Fig. 3:** Comparing of solute concentration along column with use of existing correlations with experimental values ( $Q_c=30$  lit/hr,  $Q_d=30$  lit/hr,  $N=400$  rpm, holdup=4.39%)



**Fig. 4:** Comparing of solute concentration along column with use of proposed correlation with experimental values ( $Q_c=30$  lit/hr,  $Q_d=30$  lit/hr,  $N=400$  rpm, holdup=4.39%)

Table-6 indicates the final error percentage of comparing the calculated results and experimental results for all runs.

According to mentioned table and figures, observed that using of correction factor (R) in calculating of solute concentration, error percentage is nearly high whereas using of  $D_{eff}$  in comparing with other correlations have the least error.

Therefore  $D_{eff}$  correlation for predicting of the solute concentration in different positions of column is more effective.

**Table 5:** Solute concentration along the column with use of existing correlations and proposed correlation for Run-2

L(cm)	Newman			Johnson &		Boyodzhiev		Steiner	
	C <sub>exp</sub>	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error
25	0.325	0.3532	-8.37	0.0141	95.65	0.2588	20.58	0.3011	7.58
37.5	0.165	0.2968	-78.97	0.0024	98.54	0.1862	-12.2	0.2337	-40.9
50	0.0889	0.2494	-180.5	0.0004	99.51	0.1339	-50.6	0.1813	-103
62.5	0.0632	0.2096	-231.5	0.0001	99.8	0.0963	-52.3	0.1407	-122
75	0.0377	0.1761	-366.3	6.18E-05	99.83	0.0693	-83.4	0.1092	-189
L(cm)	Lochiel & Calderbank			Davis		Temos		This work	
	C <sub>exp</sub>	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error	C <sub>cal</sub>	%error
25	0.325	0.1447	55.59	0.0839	74.23	0.3519	-8	0.244	25.11
37.5	0.165	0.0778	53.06	0.0344	79.25	0.2953	-78	0.1705	-2.8
50	0.0889	0.0418	52.89	0.0141	84.08	0.2477	-178	0.1191	-33.94
62.5	0.0632	0.0225	64.36	0.0058	90.82	0.2078	-228	0.0832	-31.5
75	0.0377	0.0121	67.95	0.0024	93.62	0.1744	-361	0.0581	-53.85

**Table 6:** Final error percentage resulted of calculated solute concentration along the column (Runs1-5)

Run	Newman	Johnson Hamielec	Boyodzhi	Steiner	Lochiel Calderba	Davis	Temos	This work
1	28.53	78.44	61.07	25.57	66.04	52.58	23.92	14.84
2	148.49	96.4	42.54	82.52	57.67	80.93	146.68	30.85
3	36.17	80.7	35.89	29.36	65.33	53.56	33.4	20.96
4	43.29	76.95	28.31	36.09	61.6	46.9	39.93	16.27
5	134.68	84.64	39.86	108.07	59.57	47.84	129.98	34.78

**Conclusions:**

Regarding to calculations made and the yielding tables and figures, the following conclusions can be made;

1- In all runs, the results of calculating column efficiency and solute concentration at different points of column and comparing them with experimental values by using of  $D_{eff}$  correlation indicates that error percentage have been decreased, therefore using of this correlation for predicting the efficiency along column and solute concentration along column is proposed.

2-By using of solute concentration prediction at different positions of column, it is possible to estimate physical properties along column, therefore accurate design of column will be extracted for calculating solute concentration along column.

**Nomenclature**

- A Column cross sectional area (m<sup>2</sup>)
- C<sub>n</sub> Taylor Constant
- C Solute concentration in dispersed phase (gr/cm<sup>3</sup>)
- C<sub>0</sub> Initial solute concentration of solute in dispersed phase (gr/cm<sup>3</sup>)
- C\* Equilibrium concentration of solute in dispersed phase (gr/cm<sup>3</sup>)
- d Drop diameter (m)
- d<sub>32</sub> Mean diameter of drop
- D<sub>d</sub> Diffusion Coefficient (m<sup>2</sup>/s)
- E Local efficiency
- D<sub>eff</sub> Effective diffusion coefficient (m<sup>2</sup>/s)
- D<sub>E</sub> Effective diffusion coefficient (m<sup>2</sup>/s)
- D<sub>OE</sub> Overall effective diffusion coefficient (m<sup>2</sup>/s)
- f<sub>v</sub> Fractional segmental volume of drop which is stagnant
- g Gravitational constant (m/s<sup>2</sup>)
- k The dimensionless number in Eq. (10) (= E<sub>oc</sub> / 6)
- K<sub>c</sub> Mass transfer coefficient based on continuous phase (m/s)
- K<sub>d</sub> Mass transfer coefficient based on dispersed phase (m/s)
- K<sub>od</sub> Overall mass transfer coefficient based on dispersed phase (m/s)

- $k_H$  Contamination coefficient which varies between 0 to 1  
 $r$  Radius direction in spherical coordinates  
 $Q_c$  Volumetric flow rate of continuous phase (cm<sup>3</sup>/s)  
 $Q_d$  Volumetric flow rate of dispersed phase (cm<sup>3</sup>/s)  
 $r_s$  Drop radius (m)  
 $R$  Internal enhancement factor for mass transfer  
 $t$  Contact time (sec)  
 $U_s$  Slip velocity of drop (m/s)  
 $U_t$  Terminal velocity of drop (m/s)

**Greek**

- $\varepsilon$  Dispersed phase holdup  
 $k$  Viscosity ratio (dispersed/continuous phase)  
 $\mu_c$  Continuous phase viscosity (Kg/m.s)  
 $\mu_d$  Dispersed phase viscosity (Kg/m.s)  
 $\lambda_n$  Eigen value  
 $\rho_c$  Continuous phase density (Kg/ m<sup>3</sup>)  
 $\rho_d$  Dispersed phase density (Kg/ m<sup>3</sup>)  
 $\Delta\rho$  Difference of dispersed and (Kg/ m<sup>3</sup>) continuous densities  
 $\gamma$  Interfacial tension (N/m)

**Groups:**

- $E_o$  Eotvos ( $gd^2 D\rho/\gamma$ )  
 $E_{oc}$  Eotvos number when drop has critical diameter  
 $U$  Velocity (m/s)  
 $Sc$  Schmidt ( $\mu / \rho D_d$ )  
 $Re$  Reynolds  $\frac{(\rho U d)}{\mu}$

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