

## A General Correlation For The Dispersed Phase Mass Transfer Coefficient For Single Drop Systems In Liquid-Liquid Extraction Columns

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The reliability of the design of any liquid-liquid extraction equipment depends upon the accuracy of the chosen correlation for the calculation of the mass transfer coefficient. However the designer is very often faced with the problem of choosing the most appropriate one, due to the great number of available correlations.

In the present work, different new correlations for the calculation of the Sherwood number for the dispersed phase are developed and tested numerically for rigid drops, circulating and oscillating drops in single drops systems and for liquid-liquid extraction packed columns. In order to take into account all the phenomena that influence the mass transfer, it is proposed to group all the dimensionless numbers that were used separately in the different existing correlations reported in the literature to end up with the following general expression:

$$Sh_d = A Re^B Fo^C Mo^D Sc_d^E We^F (1 + \mu_d/\mu_c)^G$$

The constants of this new correlation were calculated numerically for each case, and the results were compared with experimental mass transfer coefficient, where good agreements were achieved.

**Key words :** liquid-liquid extraction; mass transfer coefficient; rigid drop; circulating drop; oscillating drop; dispersed phase; packed column.

### 1. Introduction

The separation techniques such as distillation, absorption of gases, solvent extraction, adsorption, etc, are based upon the mass transfer between phases which can be liquid, vapor or solid. In most cases, one of the phases is dispersed as drops (dispersed phase) into the other one (continuous phase). The intensity of the mass exchange between phases is characterized by the mass transfer coefficient  $k$  which is generally calculated through correlations involving the Sherwood number. However these correlations are available in a great number and the choice of the most appropriate one for a given system is not an easy task. Consequently the present work aims at developing a new correlation issued from the grouping of a given set of existing ones and which tends to take into account as many specific mass transfer conditions as possible.

### 2. Theories and Correlations used

Several models and theories were developed, however these models often showed deviations from experimental results. The theories and correlations used in this present

work are: Higbie theory[1], Newman theory[2] for rigid drops with transient molecular diffusion, Kronig-Brink theory [2] for laminar diffusion with inner circulation, Handlos-Baron theory [2] for turbulent diffusion with internal turbulent circulation, Skelland and Conger correlation [3] for rigid drops, for circulating drops we used: Rozen and Bezzubova [3] correlations for average and large drops and Treybal [3] correlation, for oscillating drops we used Skelland and Conger [2] correlation and Clift et al [4] one.

### 2.1 Packed columns

Correlations and theories for single drop system quoted above can be adapted to the case of extraction columns by replacing the terminal velocity and the diameter of the single drop by the slip velocity and the average drop diameter respectively and through the hydrodynamic parameters. For this case of packed columns, the properties of the contactor appears as the packing size and its specific surface [5],[6], [7].

### 3. The calculation procedure

From the equations quoted above (and others), the great diversity of the expressions is noted. Therefore a uniform equation would be easier to use. Thus, it is proposed to use a correlation gathering all the dimensionless numbers which appear separately in existing correlations. The proposed expression for the Sherwood number of the dispersed phase is as follows:

$$Sh_d = A Re^B Fo^C Mo^D Sc_d^E We^F (1 + \mu_d/\mu_c)^G \quad (1)$$

For this purpose, a Mathcad computing program was developed for the calculation of the constants of the suggested model. The calculation procedure can be summarized as follows:

- For each case of drop behavior, an average  $Sh_d$  value is calculated by means of the various correlations used for the considered case;
- The average values of  $Sh_d$ , will be approximated by the linear model of least squares method, to obtain the constants of Equation 1.

### 4. Results and discussion

A priori, the results given by the different theories and correlations quoted above, are compared, for a system often recommended by the literature, namely Acetone/Toluene/Water, whose physical properties are summarized on the following Table 1:

**Table 1.** Physical properties of the system: acetone/toluene/water

| Physical property                             | Continuous phase | Dispersed phase |
|---|------------------|-----------------|
| Density $\rho$ (kg/m <sup>3</sup> )           | 998              | 864             |
| Viscosity $\mu$ (kg/m s)                      | 1.13 $10^{-3}$   | 5.7 $10^{-4}$   |
| Diffusion coefficient $D$ (m <sup>2</sup> /s) | 1.1 $10^{-9}$    | 2.7 $10^{-9}$   |

First we compare the use of theories and correlations cited above, the values are very varied and can be divided into two groups: one for rigid drop and with laminar circulation at the bottom and the other for drops with turbulent circulation and oscillating at the top (Figure 1). This comparison will enable to eliminate the theories and correlations which give values very different from their group average one. Thus, it is proposed to find two new correlations: one each group.

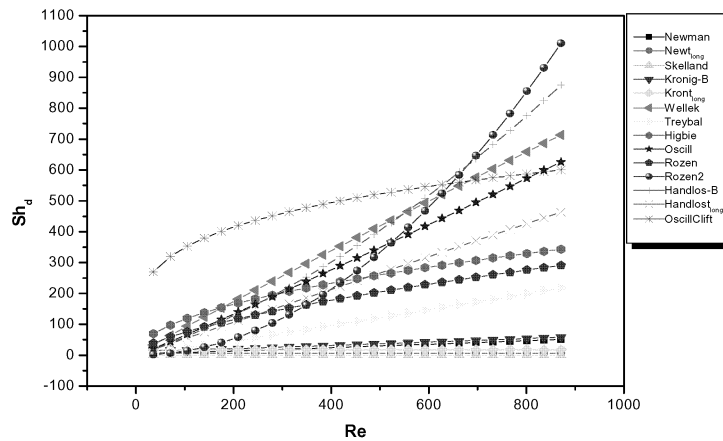


Figure 1. Comparison of existing theories and correlations

#### 4.1 New correlation for rigid and internal laminar circulating drops

For this case the two theories of Newman and Kronig-Brink are retained. These two models have already proved their reliability for this case and this stage of approximation will allow standardizing the equations to be proposed. The result given by the computing code for this case is as follows:

$$Sh_{d\_lam} = Re^{3.01} Fo^{0.438} Mo^{0.176} Sc_d^{-1.34} We^{-1.45} (1 + \mu_d / \mu_c)^{0.691} \quad (2)$$

A comparison between the new correlation and used theories is shown on Figure 2,

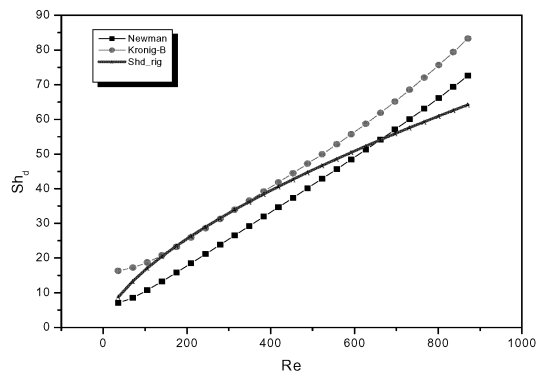


Figure 2. New correlation for rigid and internal laminar circulating drops

#### 4.2 New correlation for oscillating and internal turbulent circulation drops

From Figure 1, it can be retained for this case the following models: Handlos-Baron at long time of contact, Wellek, Treybal, Higbie, Rozen, and the correlation of Skelland for oscillating drop. As previously, an approximation of the average of these theories and correlations, leads to the following result:

$$Sh_{d\_turb} = 44.3 Re^{0.272} Fo^{0.092} Mo^{0.038} Sc_d^{0.236} We^{0.75} (1 + \mu_d/\mu_c)^{-1.34} \quad (3)$$

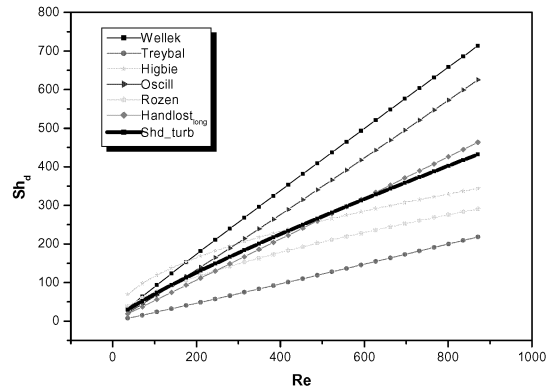


Figure 3: New correlation for oscillating and internal turbulent drops

#### 4.3 Application of the new correlations

In order to test the reliability of the proposed correlations, the results are compared with the experimental values of Table 2, for the system: Acetone/Toluene/Water, obtained in the Lehrstuhl für Thermische Verfahrenstechnik, Kaiserslautern University in Germany.

Table 2. Experimental results for: Acetone/Toluene/Water

| d (mm) | V <sub>t</sub> (m/s) | K <sub>od</sub> (m/s)   |
|--------|----------------------|-------------------------|
| 0.77   | 0.042                | 1.9 · 10 <sup>-5</sup>  |
| 1.54   | 0.07                 | 3.88 · 10 <sup>-5</sup> |
| 1.62   | 0.056                | 5.58 · 10 <sup>-5</sup> |
| 3.00   | 0.106                | 1.06 · 10 <sup>-4</sup> |

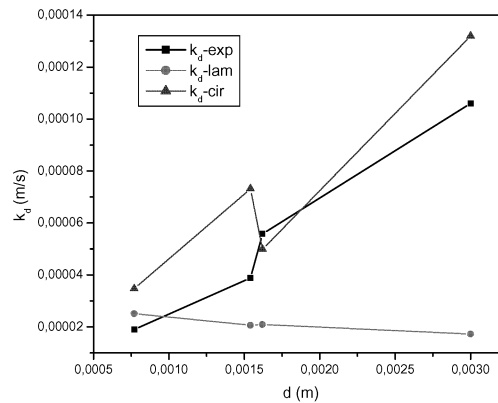


Figure 4. Experimental and calculated mass transfer coefficient

Figure 4 shows that for small drop sizes, the correlation for rigid drops give reasonable results whereas for drops with greater sizes the correlation for a drop with turbulent circulation is more adequate.

#### 4.4 Correlation for packed liquid-liquid extraction column

The obtained correlation is adapted to the case of the packed column., a similar form to that proposed by Steiner [8] for the continuous phase, is adopted. The computing code returns the results presented in Figure 4 by  $Sh_{d-olonne}$ , where the dimensions and properties of the rashig rings of the packed column are those used by Seibert and Humphrey [9], leading the following expression:

$$\frac{Sh_d - Sh_{d-turb}}{Sh_{d-turb} - Sh_{d-lam}} = 1 - \exp(2 Pe_d^{-0.12}) \quad (4)$$

Quite good agreement is noted at low Reynolds numbers only and the curves are deviating from one another as this latter is increasing.

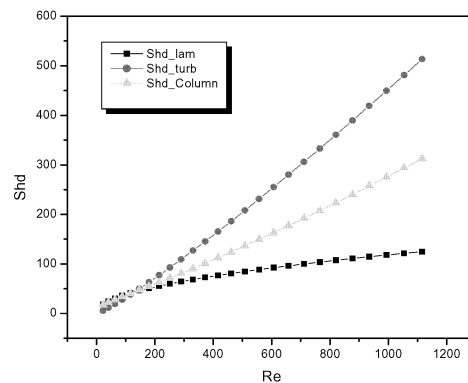


Figure 5. New correlation for packed column

## 5. Conclusion

The results of the numerical experiments carried out by the developed program code lead to three new correlations: one for single drop system with a rigid sphere behavior and internal laminar circulation, another for a drop with turbulent circulating and oscillating drops and one for the case of the extraction packed column. The proposed correlations have a uniform form, grouping a number of different correlations for the mass transfer coefficient calculation, eliminating the difficult problem of choosing the most adequate equation among the great number of available ones.

However, this study should be regarded at the preliminary stage, since further work is necessary to involve a huge number of various systems with different physical properties. Probably correction factors should be included particularly on the Schmidt number which is function of the physical properties of a given system. The developed calculation code is flexible and enables the generation of more general correlations with the availability of more experimental data for various systems.

## 6. Notation

|                |  |
|----------------|--|
| d              | : drop diameter (m)  |
| D              | : diffusion coefficient (m <sup>2</sup> /s)  |
| Fo             | : Fourier number, Dimensionless ( $4 D_d t / d^2$ )                                  |
| g              | : gravity (m <sup>2</sup> /s)  |
| k              | : mass transfer coefficient (m/s)  |
| Mo             | : Morton number, Dimensionless ( $\frac{g \Delta \rho \mu_c^4}{\rho_c^2 \gamma^3}$ ) |
| Pe             | : Peclet number, Dimensionless (Re Sc)   |
| Re             | : drop Reynolds number, Dimensionless ( $d V_t \rho / \mu$ )                         |
| Sc             | : Schmidt number, Dimensionless ( $\mu / \rho D$ )                                   |
| Sh             | : Sherwood number, Dimensionless ( $k d / D$ )                                       |
| t              | : time (s)   |
| V <sub>t</sub> | : terminal velocity (m/s)  |
| We             | : Weber number, Dimensionless ( $\frac{\rho_c V_t^2 d}{\gamma}$ )                    |

## Greek letters

|   |                                |
|---|--------------------------------|
| γ | : interfacial tension (N/m)    |
| μ | : viscosity (kg/m s)           |
| ρ | : density (kg/m <sup>3</sup> ) |

## Subscript:

|   |                    |
|---|--------------------|
| c | : continuous phase |
| d | : dispersed phase  |

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