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On The Liquid-Particle Mass Transfer Coefficient Correlation for Multiparticle Systems

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Extended Abstract

To estimate the mass transfer rate between liquid and particles, correlations for mass transfer coefficient k or its dimensionless from, the Sherwood number Sh, are generally used [1-7]. For multiparticle systems, the presence of other particles affects the mass transfer of a specific particle, and the correlations must account for this effect. In the literature, the available correlations lack rigorous theoretical support and do not consistently agree well with experimental data [2-7]. To overcome this, we propose a theoretically sound approach by using scaling and order of magnitude analysis. Based on the definition of k and the Fick's law, the order of magnitude of k and Sh are estimated as follows:

$$k\Delta C \sim D \Delta C/\delta_c \rightarrow k \sim D/\delta_c \rightarrow \text{Sh} \sim d_p/\delta_c$$
 (1)

Here, D is the solute diffusivity, ΔC is the concentration difference between the particle surface and the liquid bulk, δ_c is the length scale for significant concentration changes near the particle surface, and d_p is the particle diameter. Because of the large Schmidt number Sc in the liquid, provided the Reynolds number Re is not extremely small, the Peclet number Pe is far larger than unity. In this case, a thin concentration boundary layer forms around the particles, and δ_c is its thickness [8]. δ_c is very small, and this allows us to simplify the mass balance equations for the liquid and the solute within this boundary layer. Scaling these simplified equations yields the relation between δ_c and the velocity scale at the outer edge of the concentration boundary layer, denoted by u_c . This relation is:

$$\frac{\delta_c}{d_p} \sim \left(\frac{D}{u_c d_p}\right)^{1/2} \tag{2}$$

Moreover, δ_c and u_c can be linked to the length and velocity scales for the velocity field around the particles, denoted as δ_v and u_v . Due to the large Sc, Pe is much larger than Re, and thus we can assume that δ_c is much smaller than δ_v . Using the scaling method, we then obtain the following equation:

$$\frac{\delta_c}{\delta_v} \sim \frac{u_c}{u_v} \to \frac{\delta_c}{d_p} \sim \left(\frac{D}{u_v d_p} \frac{\delta_v}{d_p}\right)^{1/3} \tag{3}$$

 δ_v and u_v can be estimated by order of magnitude analysis of the drag force acting on a particle F_p . For a uniform suspension at equilibrium, F_p features the unhindered terminal velocity u_t through the following equation [9]:

$$F_p = \left(\frac{\pi}{4} d_p^2\right) \left(\frac{1}{2} \rho_e u_t^2\right) C_D^t \tag{4}$$

Here, ρ_e is the liquid density, while C_D^t is the particle drag coefficient characterized by u_t . This coefficient can be calculated with the Dallavalle correlation [10], given by:

$$C_D^t = \left(0.63 + 4.8 \text{Re}_t^{-1/2}\right)^2, \text{ Re}_t \equiv \rho_e u_t d_p / \mu_e$$
 (5)

where μ_e is the liquid viscosity and Re_t is the Reynolds number characterized by u_t . u_t can be related to the superficial velocity u by the following equation [11]:

$$u = u_t \varepsilon^n, n = \frac{4.8 + 2.4 \cdot 0.175 \text{Re}_t^{3/4}}{1 + 0.175 \text{Re}_t^{3/4}}$$
 (6)

where ε is the void fraction. Furthermore, F_p can be estimated by:

$$F_p \sim \left(\mu_e \frac{u_v}{\delta_v}\right) \pi d_p^2 \tag{7}$$

For multiparticle systems, we can assume that u_v has the same order of magnitude as the interstitial velocity u/ε . Accordingly, using Eqs. (2-7), we obtain:

$$\frac{\delta_c}{d_p} \sim 2 \left(\frac{D}{u d_p} \frac{\varepsilon^n}{\text{Re}_t C_D^t} \right)^{1/3}, \text{Pe} \gg 1$$
 (8)

Since the concentration boundary layer theory was used, Pe is required to be much larger than unity. Finally, using Eq. (1) and introducing a constant C, expected to have unit order of magnitude, the correlation for Sh is given by:

$$Sh = \frac{c}{2} \varepsilon^{-2n/3} \left(0.63 \text{Re} + 4.8 \text{Re}^{1/2} \varepsilon^{n/2} \right)^{2/3} \text{Sc}^{1/3} , \text{ Re} \equiv \rho_e u d_p / \mu_e , \text{ Pe} \gg 1$$
 (9)

C is estimated by matching Eq. (9) with experimental data from packed and fluidized beds [12-19]. The obtained value has unit order of magnitude, and the correlation agrees well with experimental data, with errors less than 30%. These results verify the applicability of the newly proposed approach.

References

- [1] R. B. Bird, Transport phenomena, John Wiley & Sons, 2002.
- [2] T. Kataoka, H. Yoshida, K. Ueyama, Mass transfer in laminar region between liquid and packing material surface in the packed bed, *J. Chem. Eng. Japan*, 5 (1972) 132–136.
- [3] Y. Kawase, J. J. Ulbrecht, A new approach for heat and mass transfer in granular beds based on the capillary model, *Ind. Eng. Chem. Fundam.*, 24 (1985) 115–116.
- [4] R. Pfeffer, J. Happel, An analytical study of heat and mass transfer in multiparticle systems at low Reynolds numbers, *AIChE. J.*, 10 (1964) 605–611.
- [5] M. Satish, J. Zhu, Flow resistance and mass transfer in slow non-Newtonian flow through multiparticle systems, *J. Appl. Mech.*, (1992).
- [6] P. K. Agarwal, Transport phenomena in multi-particle systems—ii. particle-fluid heat and mass transfer, *Chem. Eng. Sci.*, 43 (1988) 2501–2510.
- [7] F. Scala, Particle-fluid mass transfer in multiparticle systems at low Reynolds numbers, *Chem. Eng. Sci.*, 91 (2013) 90-101.
- [8] L. A. Belfiore, Transport phenomena for chemical reactor design, John Wiley & Sons, 2003.
- [9] L. Mazzei, P. Lettieri, A drag force closure for uniformly dispersed fluidized suspensions, *Chem. Eng. Sci.*, 62 (2007) 6129–6142.
- [10] J. M. Dallavalle, Micromeritics: the technology of fine particles, 1948.
- [11] J. Richardson, W. Zaki, Sedimentation and Fluidization: Part I, Trans. Insti. Chem. Eng., 1954.
- [12] L. K. McCune, R. H. Wilhelm, Mass and momentum transfer in a solid-liquid system, *Ind. Eng. Chem. Res.*, 41 (1949) 1124–1134.
- [13] B. J. Gaffney, T. B. Drew, Mass transfer from packing to organic solvents in single phase flow through a column., *Ind. Eng. Chem. Res.*, 42 (1950) 1120–1127.
- [14] I. Toshio, D. ohtake, tadayoshi Okada, Mass transfer in packed bed, *Chem. Mach.*, 15 (1951) 255–261.
- [15] W. Dunn, C. Bonilla, C. Ferstenberg, B. Gross, Mass transfer in liquid metals, AIChE. J., 2 (1956) 184–189.
- [16] J. Williamson, K. Bazaire, C. Geankoplis, Liquid-phase mass transfer at low Reynolds numbers, *Ind. Eng. Chem. Fundam.*, 2 (1963) 126–129.
- [17] E. Wilson, C. Geankoplis, Liquid mass transfer at very low Reynolds numbers in packed beds, *Ind. Eng. Chem. Fundam.*, 5 (1966) 9–14.
- [18] S. N. Upadhyay, G. Tripathi, Liquid-phase mass transfer in fixed and fluidized beds of large particles, *J. Chem. Eng. Data*, 20 (1975) 20–26.
- [19] A. Livingston, J. Noble, Mass transfer in liquid—solid fluidized beds of ion exchange resins at low Reynolds numbers, *Chem. Eng. Sci.*, 48 (1993) 1174–1178.