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Correlation for the Mass Transfer Coefficient between Liquid and Particles in Multiparticle Systems

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Extended Abstract

To assess the mass transfer rate between liquid and particles, correlations involving the mass transfer coefficient k or its dimensionless counterpart, the Sherwood number Sh, are commonly employed [1-7]. In the context of multiparticle systems, the presence of other particles affects the mass transfer of a specific particle, and therefore correlations must account for this effect. The available correlations lack rigorous theoretical support and do not always agree with experimental data [2-7]. In this work, we propose a theoretically robust approach based on scaling and order of magnitude analysis. Using the definition of k and Fick's law, we estimate the order of magnitude of k and Sh as follows:

$$k\Delta C \sim D\,\Delta C/\delta_c \rightarrow k \sim D/\delta_c \rightarrow \mathrm{Sh} \sim d_p/\delta_c \tag{1}$$

where D is the solute molecular diffusivity, ΔC is the concentration difference between the particle surface and the bulk of the liquid, δ_c is the length scale for significant concentration changes near the particle surface, and d_p is the particle diameter. Due to the large Schmidt number (Sc) in the liquid, when the Reynolds number (Re) is not extremely small, the Peclet number (Pe) is much larger than unity. In such cases, a thin concentration boundary layer forms around the particle, δ_c representing its thickness [8]. Given that δ_c is very small, we can simplify the mass balance equations for the liquid mixture and the solute within this boundary layer. Scaling these simplified equations yields a relationship between δ_c and the velocity scale u_c at the outer edge of the concentration boundary layer; this relationship reads:

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

Now, we relate δ_c and u_c to the length and velocity scales of the velocity field around the particles, denoted as δ_v and u_v, respectively. Due to the large Sc and to Pe being far larger than Re, we can assume that δ_c is far smaller than δ_v. Employing the scaling method, we can write:

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

To estimate δ_v and u_v, we employ the order of magnitude analysis applied to the drag force acting on a particle (F_p). For a uniform suspension at equilibrium, F_p is related to the unhindered terminal velocity (u_t) through the equation [9]:

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

where ρ_e is the liquid density and C_D^t is the particle drag coefficient characterized by u_t. To calculate C_D^t, we employ the correlation of Dallavalle [10]:

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

where μ_e is the liquid viscosity. u_t can be related to the superficial velocity (u) by the equation [11]:

$$u = u_t\varepsilon^n \quad \text{with } n = \frac{4.8+2.4\cdot 0.175\mathrm{Re}_t^{3/4}}{1+0.175\mathrm{Re}_t^{3/4}} \tag{6}$$

Moreover, F_p can be estimated as:

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

For multiparticle systems, assuming u_v has the same order of magnitude as the interstitial velocity u/ε and using Eqs. (2) to (7), we obtain:

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

Given the application of concentration boundary layer theory, Pe must be significantly larger than unity. Finally, utilizing Eq. (1) and introducing a constant C (expected to be of unit order of magnitude), the correlation for Sh reads:

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

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

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