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Empirical correlations for axial dispersion coefficient and Peclet number in fixed-bed columns

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ABSTRACT

In this work, a new correlation for the axial dispersion coefficient was obtained using experimental data in the literature for axial dispersion in fixed-bed columns packed with particles. The Chung and Wen correlation, the De Ligny correlation are two popular empirical correlations. However, the former lacks the molecular diffusion term and the latter does not consider bed voidage. The new axial dispersion coefficient correlation in this work was based on additional experimental data in the literature by considering both molecular diffusion and bed voidage. It is more comprehensive and accurate. The Peclet number correlation from the new axial dispersion coefficient correlation on the average leads to 12% lower Peclet number values compared to the values from the Chung and Wen correlation, and in many cases much smaller than those from the De Ligny correlation.

1. Introduction

Axial dispersion in a fixed-bed packed with particles is important in mass transfer in many applications in areas such as adsorption, liquid chromatography and hydrology [1]. Axial dispersion in a fixed-bed column is caused by molecular diffusion and turbulent mixing around particles [2,3]. A model for dispersion processes in porous media is usually based on convective-diffusion and the mean solute concentration in the bulk-fluid phase (C_b), the mean interstitial velocity of fluid (v), the source term (S_b), the axial dispersion coefficient (D_b) and time (t) [2,4]. Peclet (Pe) number for nondimensionalization in analytical and numerical solutions is sometimes used in axial dispersion models. It reflects the characteristic ratio of convective transport rate to diffusive transport rate. The Pe term is sometimes dropped for simplicity. However, this practice often leads to abnormally sharp or shockwave profiles [5]. In numerical solutions, it is beneficial to retain the Pe term for solution stability. In liquid chromatography simulation, some researchers [3,5,6] have noticed that the Pe_L (Peclet number based on the bed length) values estimated from existing empirical correlations tend to be very large and yield much sharper concentration profiles than experimental profiles. Gu and Zheng [7] artificially used $Pe_L = 1000$ for simulation to fit experimental data because the estimated Pe_L was too large and caused numerical difficulties. Thus, it is desirable to revisit the estimation of Pe_L.

The popular Chung and Wen correlation [8] was first published in 1968 by correlating large amounts of experimental data. It did not consider the molecular diffusion because it suggested that D_b was usually one or two orders of magnitude higher than molecular diffusivity [3]. In 1970, De Ligny [1] incorporated molecular diffusion that comes from Langer et al. [9] based on the turbulent mixing term from Giddings' random-walk analysis. However, his correlation used a fixed bed voidage of $\varepsilon_b = 0.4$, which limits its application. Other researchers [10–12] published additional axial dispersion coefficient (D_b) correlations using experimental data. However, these new correlations did not gain popularity due to various reasons such as increased complexity [13] or no improvement in accuracy.

It is desirable to obtain an updated axial dispersion coefficient correlation (D_b) that considers both molecular diffusion coefficient (D_m) and bed voidage (ε_b) based on the large amount of experimental data used by Chung and Wen and additional published data in the literature. A new correlation based on more experimental data can improve accuracy in the estimation of Pe_L.

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2. Mathematical correlation

The primary mechanisms that contribute to axial dispersion in a fixed bed are molecular diffusion and turbulent mixing due to merging and splitting of flows around the particles [14]. It is now generally agreed that the effects of diffusion and convection are "coupled" in the axial dispersion of matter by fluid flow through fixed beds [15].

Eq. (1) represents the classical correlation that combines the contribution of eddy diffusion and molecular diffusion using the coupling theory in the absence of mass transfer between a mobile phase and stationary phase [14,15],

$$\frac{1}{Pe_p} = \frac{D_b}{d_p\nu} = \frac{\lambda}{1 + CD_m/(d_p\nu)} + \frac{\gamma D_m}{(d_p\nu)} \tag{1}$$

where γ, λ and C are dimensionless coefficients, depending on the geometry of the column packing and the flow rate, Pe_p is the Pe number based on the particle diameter ($\nu d_p/D_b$), d_p the particle diameter, ν the interstitial velocity [9,16]. Eq. (1) can be rearranged to yield Eq. (2),

$$D_b = \gamma D_m + \frac{\lambda d_p \nu}{1 + CD_m/(d_p\nu)} \tag{2}$$

Eq. (2) can be nondimensionalized using dimensionless Pe_p, Reynolds number defined by ($Re = 2R_p\nu\varepsilon_b\rho/\mu$) using the superficial velocity and Schmidt number defined by $Sc = \mu/(D_m\rho)$ as shown in Eq. (3). Note that in mass transfer correlations, Re is often defined using superficial velocity ($\nu\varepsilon_b$) instead of interstitial velocity (ν).

$$\frac{1}{Pe_p} = \frac{\varepsilon_b\gamma}{ReSc} + \frac{\lambda}{1 + \frac{\varepsilon_b C}{ReSc}} \tag{3}$$

Based on Eq. (2), one of the popular correlations is the Chung and Wen empirical correlation after dropping the molecular diffusion term by considering only eddy diffusion [8]:

$$D_b = \frac{2R_p\nu\varepsilon_b}{0.2 + 0.011Re^{0.48}} \qquad \left(10^{-3} < Re < 10^{3}\right) \tag{4}$$

where R_p is particle radius. Using the Pe_p number, Eq. (4) converts to Eq. (5) as follows,

$$\varepsilon_b Pe_p = 0.2 + 0.011Re^{0.48} \tag{5}$$

Note that Pep here uses the D_b in Eq. (4) that considers only eddy diffusion while ignoring molecular diffusion (i.e., $D_m = 0$).

Based on Eq. (2), De Ligny [15] obtained the following empirical correlation for D_b for liquid flow in packed beds with spherical particles,

$$D_b = 0.7D_m + \frac{5R_p\nu}{1 + 4.4D_m/(R_p\nu)} \tag{6}$$

Using Pe_p, Eq. (6) yields Eq. (7),

$$1/Pe_p = \frac{0.7D_m}{2R_p\nu} + \frac{1}{0.4 + 1.76D_m/(R_p\nu)} \tag{7}$$

The molecular diffusion coefficient (D_m) in Eq. (7) can be estimated based on the solute's molecular weight (M_W) using the following correlation from Polson [14]:

$$D_m\left(m^2\cdot s^{-1}\right) = 2.74\times 10^{-9}(M_W)^{-1/3} \qquad (M_W > 1000) \tag{8}$$

In this work, the following correlation form was first used to update the Chung and Wen correlation for the fix bed condition,

$$\varepsilon_b Pe_p^* = x_1 + x_2 Re^{x_3} \tag{9}$$

where $Pe_p{}^* = \nu d_p/D_b{}^*$ and $D_b{}^*$ is the axial dispersion coefficient that considers only eddy diffusion and ignores molecular diffusion.

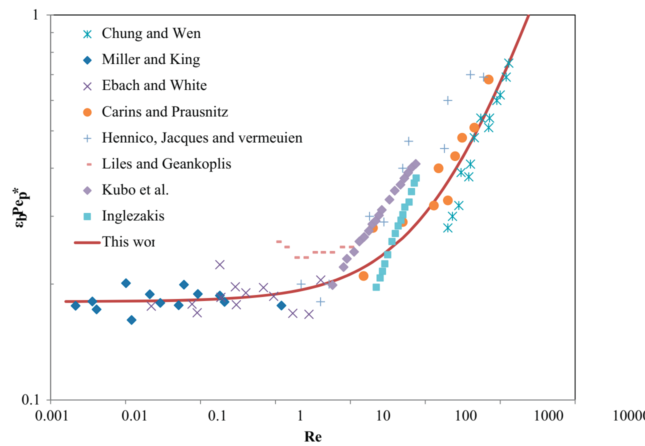

Fig. 1. Correlating experimental data to obtain Eq. (12).

Thus, the new D_b correlation in this work was obtained using Eq. (10) inspired by Eq. (6),

$$D_b = 0.7D_m + D_b^* \tag{10}$$

$D_b{}^*$ is shown as the second term on the right hand side of Eq. (11) based on Eq. (6),

$$D_b = 0.7D_m + \frac{2R_p\nu\varepsilon_b}{x_1 + x_2Re^{x_3}} \tag{11}$$

in which the $D_b{}^*$ term adopted Eq. (4) form. The correlation parameters x_1, x_2, x_3 were obtained through experimental data fitting using MATLAB (Version R2014a).

3. Results and discussions

3.1. Peclet number correlation

Eq. (12) was obtained from fitting experimental data sets in the literature using MATLAB (R2014a). This is a new empirical relationship between Peclet number and Reynolds number, which considers eddy diffusion while ignoring molecular diffusion.

$$\varepsilon_b Pe_p^* = 0.18 + 0.008Re^{0.59} \tag{12}$$

It is customary in chemical engineering literature to present dispersion data as graphs of the logarithm of the Peclet number vs. the logarithm of the Reynolds number. Fig. 1 shows the double-log plot of experimental data [17–23] and Eq. (12). In the creeping flow for obtaining a conservative upper estimate for the convective dispersion coefficient, the Miller and King [17] data and also Ebach and White [18] data including experiment with rings, Berl saddles, Intalox saddles were used. Additionally, there were some reports for the creeping flow regime in the literature but some of them were deemed not adoptable because they used narrow columns or had large errors in the measured dispersion coefficients [10].

Fig. 2 shows the Chung and Wen correlation [8] and its comparison with the same experimental data in Fig. 1. Figs. 1 and 2 show that the new correlation fitted the experimental data slightly better than the Chung and Wen correlation in both lower and higher Re regions.

It should be noted that Chung and Wen correlation were based on both fixed bed and fluidized bed data in the literature, while the new empirical correlation in this work aimed at finding a better correlation for fixed-bed columns. The new correlation is particularly suited for liquid chromatography modeling.