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Determination of dynamic dispersion coefficients for passive and reactive particles flowing in a circular tube

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ABSTRACT

Using the moment analysis method and the Green's function, mathematical formulations valid across the full-time scale have been derived to determine dynamic dispersion coefficients for passive and reactive particles flowing in a circular tube with fully-developed laminar flow under different source conditions. The newly proposed formulations were verified through agreements with both analytical solutions and random walk particle tracking (RWPT) simulations. The relationship between particle size and dispersion coefficient for passive particles varies with time and they are positively correlated if Peclet number is larger than its critical value; otherwise, they are negatively correlated. Furthermore, the critical Peclet number decreases as time increases. Compared to an instantaneous point source, the critical Peclet number for a volumetric planar source is much smaller. At a small size ratio, size-exclusion effects on passive particle dispersion can be neglected across the full-time scale for both instantaneous point and volumetric planar sources; whereas, at a large size ratio, its significance needs to be considered, depending upon time and source condition. Using $D_{\mathrm{re\_diff}} = 0.02$ ($D_{\mathrm{re\_diff}} = (D - D_{\mathrm{non\_ad}})/D$, where D and $D_{\mathrm{non\_add}}$ are dispersion coefficients with and without axial diffusion, respectively) as the critical value, axial-diffusion effects on dispersion are negligible for passive solutes at long times if Peclet number is not smaller than 50; however, due to size exclusion this is not applicable for passive particles. At early times, reaction rate, center-of-mass velocity, and dispersion coefficient are not sensitive to Damköhler number for reactive particles. At long times, reaction rate and enter-of-mass velocity increases in magnitude as the Damköhler number increases, while the dispersion coefficient decreases with increasing Damköhler number. Consequently, reaction at the tube walls greatly affects concentration distributions.

1. Introduction

Quantification and understanding of dispersion behaviour of solutes and particles in porous media are of significance in various applications including enhancing oil recovery, assessing environment risk, and performing chromatography analysis [1–3]. Mathematical models at microscopic and macroscopic scales describe solute and particle transport in porous media. Compared to a microscopic model, a macroscopic model is simpler and more convenient; however, it fails to provide insight into intrinsic controlling factors and fundamental mechanisms [4,5]. Pore network models, where the porous medium is represented by the interconnected pores and tubes, have been widely used to characterize fluid flow in porous media [4,6–8]. On the other hand, the tube-bundle model, which assumes the porous medium to be an assemblage of tubes, is also widely used for describing fluid flow in porous media [2,9]. Consequently, it is important to quantify such dispersion problems in a circular tube, which serve as the foundation to quantify solute and particle transport phenomena in porous media.

Since Taylor's pioneering work [10], numerous efforts have been made to quantify dispersion of passive (i.e., nonreactive) solutes in a fully-developed laminar tube flow [11–18]. Although the contribution of axial diffusion to solute dispersion was neglected in Taylor's original work [10], it was subsequently considered by Aris [11]. Ananthakrishnan *et al.* [13] numerically showed that axial diffusion is important when Peclet number ($N_{\mathrm{Pe}} = \bar{v}R/D_{\mathrm{m}}$, where $\bar{v}$ is the average flow velocity, R is the tube radius; and D_{m} is the molecular diffusion coefficient) is less than about 50; and at low N_{Pe}, its significance varies, depending upon dimensionless time ($t_{\mathrm{D}} = t/\tau$, where t is the elapsed time and $\tau = R^2/D_{\mathrm{m}}$). Compared to passive solutes, few attempts have been extended to determine dispersion coefficients of passive particles flowing in a circular tube, although solutes and particles disperse differently [19–22]. Considering the size-exclusion effects of particles, James and Chrysikopoulos [23] proposed a mathematical model to quantify the asymptotic dispersion process of passive particles flowing in a circular tube.

The moment analysis method proposed by Aris [11] has been widely

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Nomenclature

Notation

c	Solute concentration, M/L^3
c_0	Initially injected solute concentration, M/L^3
c_m	Transverse average concentration, M/L^3
C_n	The n^{th} local axial moments
d_p	Particle diameter, L
d_{p_crit}	Critical particle diameter, L
d_{tube}	Tube diameter, L
D	Dispersion coefficient, L^2/t
D_m	Molecular diffusion coefficient, L^2/t
D_{no}	Dispersion coefficient without size-exclusion effect, L^2/t
D_{non_ad}	Dispersion coefficient without axial diffusion, L^2/t
D_{re_diff}	Relative difference in dispersion coefficient with and without axial diffusion $D_{re\ diff}$ = (D − Dnon ad)/D
J_n	The n^{th} order Bessel function of the first kind
k	Boltzman's constant, ML^2/t^2/T
k_s	Irreversible absorption rate, L/t
K_0	Reaction rate, 1/t
m_n	The n^{th} global moments
N_{Pe}	Peclet number ($N_{Pe} = \bar{v}R/D_m$), dimensionless
N_{Pe_crit}	Critical Peclet number, dimensionless
r	Radial distance from the tube centerline, L
r_d	Size ratio of tube diameter and particle diameter ($r_d = d_p/d_{tube}$), dimensionless
r_d	Radial distance from the tube centerline ($r_d = r/(R-0.5d_p)$), dimensionless
r'	Radial distance of injection location from the tube centerline, L
R	Tube radius, L
t	Elapsed time, t
Δt	Time step, t
t_D	Dimensionless time $t_D = t/\tau$
T	Absolute temperature, T
v	Flow velocity, L/t
v_c	Center-of-mass velocity, L/t
v_{max}	Maximum flow velocity, L/t
$\bar{v}$	Average flow velocity, L/t
x	Coordinate parallel to the tube wall as shown in Fig. 1, L
X	$X(t) = \int_0^t v_c(t)dt$ as shown in Eq. (11), L
y	Coordinate perpendicular to the tube walls as shown in Fig. 1, L
z	Coordinate perpendicular to the tube walls as shown in Fig. 1, L

Greek letters

α_n	Roots of $J_1(\alpha_n) = 0$ or $\alpha_n J_1(\alpha_n) - \beta J_0(\alpha_n) = 0$, dimensionless
β	Damköhler number, dimensionless
δ	Dirac delta function, dimensionless
ζ	$\zeta(t) = \int_0^t K_0(t)dt$ as shown in Eq. (11), dimensionless
η	Fluid dynamic viscosity, Ft/L^2
ξ	$\xi(t) = \int_0^t D(t)dt$ as shown in Eqn. (11), L^2
ρ	Normalized density function, dimensionless
τ	Critical time $\tau = (R-0.5d_p)^2/D_m$, t

used to describe transport behaviour because the concentration moments can provide information about concentration evolution. The first three moments respectively relating to the conservation of injected mass, effective displacement, and solute dispersion are usually used to describe the distribution of transverse average concentration with the aid of the Taylor dispersion model [24]. Regarding reactive solutes flowing in a circular tube, Sankarasubramanian and Gill [25] developed a dispersion model including the effects of first-order irreversible reaction at the walls. Due to the complexity of the problem, however, only asymptotic expressions for the reaction rate (K_0), center-of-mass velocity (v_c), and dispersion coefficient (D) were derived. Using the Chatwin's expansion method [14], Barton [26] extended the results of Sankarasubramanian and Gill [25] to derive more exact asymptotic expressions for K_0, v_c, and D, showing good agreements with numerical results. Assuming that mass flux at the walls depends linearly upon concentration at earlier times, Purnama [27] extended Taylor's theory to determine D for reactive solutes after sufficiently long times. Considering first-order irreversible reaction at the walls, Das and Mazumder [28] described the temporal evolution of D for reactive solutes using numerical solutions. Taking both reversible and irreversible first-order reactions at the walls into account, Ng and Rudraiah [29] derived asymptotic equations for K_0, v_c, and D. Considering continuity of concentration and mass flux as boundary conditions, Dejam *et al.* [30] developed an asymptotic equation for D. Incorporating the effects of London, Van der Waals, viscous, and Debye double layer forces, Brenner and Gaydos [31] proposed theoretical formulations to calculate v_c and D for reactive particles following in a circular tube after sufficiently long times. So far, no attempt has been made to determine dispersion coefficients for passive particles flowing in a circular tube across the full-time scale under different source conditions, and the effects of particle size and axial diffusion remain unknown. In addition, it is desired to not only develop analytical equations to determine K_0, v_c, and D for reactive particles flowing in a circular tube across the full-time scale, but also examine the effects of the aforementioned three parameters on particle concentration distribution.

In this study, mathematical formulations have been developed to determine dynamic dispersion coefficients for passive particles flowing in a circular tube under fully-developed laminar flow subject to different source conditions. The effects of particle size and axial diffusion on passive particle dispersion have been thoroughly examined. For reactive particles, the first-order irreversible reaction is considered to derive analytical equations for K_0, v_c, and D across the full-time scale. The modified Taylor dispersion model proposed by Sankarasubramanian and Gill [25] is used to examine the effects of K_0, v_i, and D on particle concentration distributions. The local moment analysis method and Green's function are employed, while random walk particle tracking (RWPT) algorithm is used to verify the newly derived formulations.

2. Theoretical formulations

Fig. 1 shows schematic diagrams for passive and reactive particles transport in a circular tube with semi-infinite length. In this study, the effects of size-exclusion are considered to differentiate solute and particle dispersion, thus the widely adopted assumptions for solute dispersion are considered. Mathematical formulations are derived based on the following assumptions: (1) flow is axisymmetric, fully-developed, and laminar; (2) dispersion is isothermal; (3) molecular diffusion is independent of concentration [10–13,15,17,18,32–36]; (4) particles are neutrally buoyant and travel at their centroid velocity; (5) no reactions for passive particles [20,22,23]; and (6) first-order irreversible reaction occurs between reactive particles and tube walls.