

LONGITUDINAL DISPERSION COEFFICIENT CALCULATION DURING MISCIBLE FLOW IN HETEROGENEOUS POROUS MEDIA USING PORE SCALE SIMULATION

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This paper was prepared for presentation at the International Symposium of the Society of Core Analysts held in Snowmass, Colorado, USA, 21-26 August 2016

ABSTRACT

Miscible recovery techniques are among the most efficient and widely used enhanced oil recovery methods both in conventional and in heavy oil reservoirs (miscible gas flooding and solvent injection, respectively). The efficiency of a miscible flood is significantly dependent on the degree of mixing that occurs between the fluids. Mixing of the injected gas/solvent with oil leads to solvent dilution and thus reduces the effective strength of miscible displacement. The primary mechanisms of miscible mixing in pore space are molecular diffusion and convection (mechanical spreading) due to bulk flow velocity. The combined effect of these two mechanisms on the degree of mixing can be characterized by the dispersion coefficient. Laboratory measurement of this parameter is difficult due to the fact that it is strongly dependent on flow and porous media properties. An alternative approach is to numerically calculate dispersion coefficient using pore scale digital core analysis. In this study, pore level miscible displacements in heterogeneous porous media are computationally modeled through simultaneous solving of Navier-Stokes, Continuity, and Convection-Diffusion equations on virtual unconsolidated granular porous media. These virtual media are constructed by a pattern generator using the concept of random packing of grains. The heterogeneity level of these media is characterized by a coefficient of variations defined as the ratio of standard deviation in grain diameter to the mean grain diameter. Using the results of numerical simulations, longitudinal (along the flow direction) dispersion coefficient is calculated at different values of flow velocity, viscosity ratio, and pore scale medium heterogeneity. The input diffusion coefficients are either constant or functions of concentration. The results of the simulations show that when viscosity ratio is unity, at very low Peclet numbers the dominant transport mechanism is molecular diffusion. At high Peclet numbers, however, advection is dominant and the magnitude of longitudinal dispersion coefficient scales with $N_p^{1.2}$. Higher heterogeneity of media will result in higher values of longitudinal dispersion coefficient. Also, it is found that using an appropriate average diffusion coefficient over the range of concentration interval can adequately account for concentration dependency of diffusion coefficient. The effect of viscosity contrast on

longitudinal dispersion coefficient is shown to be significant. Viscous fingering due to an unfavorable viscosity ratio leads to higher values for longitudinal dispersion coefficient.

INTRODUCTION

Miscible displacement and mixing of fluids in porous media is of fundamental importance in many natural processes and engineering applications, including but not limited to enhanced oil recovery [1,2], environmental remediation [3-6], and CO₂ sequestration [7]. Fluids mixing in porous media is the combined result of molecular diffusion due to Brownian motion of fluid particles, as well as mechanical dispersion caused by interstitial flow velocity and its variations (both in magnitude and direction) due to medium heterogeneity.

The level of mixing in porous media is generally quantified by dispersion coefficient. In the past, dispersion coefficient has been used extensively to quantify the degree of mixing during miscible flows in porous media, both theoretically and experimentally. Taylor [8] and later Aris [9,10] investigated the viscous flow of a soluble matter in a fluid flowing through a straight circular capillary tube and theoretically described the degree of mixing by an effective dispersion coefficient. Brigham et al. [11] used glass bead packs and natural cores to investigate the effect of various parameters on the dispersion coefficient and degree of mixing through miscible displacement experiments. Perkins and Johnston [12] discussed the effect of molecular diffusion and dispersion on miscible flows and summarized information and interpretations from previous literature on miscible fluids. Coelho et al. [13] numerically obtained the values of dispersion coefficient in random spherical packings and concluded that their results were in a good agreement with experiments in consolidated sandpacks and sands. Transient and asymptotic dispersion coefficients have been calculated in regular and random sphere packings by using random-walk particle tracking and Lattice-Boltzmann methods to model solute transport and fluid flow, respectively [14]. Bijeljic et al. [15] used pore scale network simulation to calculate dispersion coefficient in a diamond lattice of throats representing Berea sandstone. Beard and Wu [16] presented an analytical dispersion coefficient for the flow of solute inside a system of capillary tubes with randomly assigned velocities. Pore scale simulations also have been used to study dispersion phenomena in porous media. Garmeh et al. [17] explored different aspects of mixing in porous media by numerical simulations at the pore scale in series and layered heterogeneous porous media constructed by different arrangements of circular grains. Their numerical results were in agreement with classical relationship between dispersion coefficient and velocity reported by [12]. Mostaghimi et al. [18] used direct images of porous media obtained from microcomputed tomography scan of rock cores and simulated flow and transport on these images using a Stokes solver for flow modeling and a streamline-based algorithm for solute transport. They were able to accurately predict the available data for longitudinal dispersion coefficient in the literature. Taheri et al. [19] developed a sub pore scale modeling approach based on numerical methods and investigated the values of dispersion coefficient during miscible displacement in several images of micro-models with different properties.

The rate of mixing and magnitude of dispersion coefficient during miscible displacement in porous media is strongly dependent on medium heterogeneity and viscosity ratio of fluids. Presence of microscale/macroscale heterogeneities results in preferred paths for fluid particles to move and thus channeling of flow. An unfavorable viscosity ratio also gives rise to instabilities at the leading edge of concentration profile and subsequently results in viscous fingering. This heterogeneity induced channeling and viscous fingering will increase the size of miscible mixing zone and consequently the magnitude of dispersion coefficient. The experimental works of [20] and [21] on glass bead columns demonstrated that increasing the variance of bead size resulted in higher dispersion rates. Experimental study of dispersion tests by [11] on random bead packs showed that higher dispersion coefficients were encountered during flow and transport at higher viscosity ratios. Bretz et al. [22] used thin sections to analyze porous medium heterogeneity and experimentally measured higher dispersion coefficient for wider pore size distributions. Numerical simulations of [23] and [24] on heterogeneous permeability fields demonstrated that increasing macroscale heterogeneity of medium in terms of Dykstra-Parson's (DP) coefficient will lead to higher dispersion coefficients. Garmeh and Johns [25] conducted numerical simulations of miscible displacement on correlated permeability fields to predict the values of dispersivities (dispersion coefficient normalized by flow velocity) at different levels of macroscale medium heterogeneity and viscosity ratio. They concluded that an increase in medium's heterogeneity (in terms of DP coefficient) and viscosity ratio results in higher values of dispersivity.

In this study, miscible displacements in two dimensional heterogeneous porous media are simulated through simultaneous solving of Navier-Stokes, continuity, and convection-diffusion equations in pore scale. Two dimensional packings of grains with different levels of microscale (local) heterogeneity are reconstructed using a pattern generator package developed by [1]. These media are constructed by random packing of circular grains with different diameters randomly taken from a particle size distribution (PSD). The heterogeneity level of these media is characterized by a coefficient of variations defined as the ratio of standard deviation in grain diameter to the mean grain diameter. Through this study, the effects of viscosity ratio and pore scale heterogeneity of porous media on the values of dispersion coefficient during miscible displacement at different Peclet numbers (flow velocities) are investigated. Both constant and concentration-dependent molecular diffusion coefficients are considered here to investigate how it affects the results.

METHODOLOGY

Governing Equations

We model miscible displacement in pore scale by solving flow and transport equations together. In order to achieve that, three equations of continuity, Navier-Stokes, and convection-diffusion (Eqs.1-3, respectively) are solved numerically using commercially available code COMSOL multi-physics:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p \mathbf{I} + \mu \nabla \mathbf{u}] \quad (2)$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c) + \mathbf{u} \cdot \nabla c = 0 \quad (3)$$

In the above equations, ρ is mixture density, \mathbf{u} is pore velocity vector, p is pressure, μ is mixture viscosity, c denotes the concentration of solute in displacing fluid, and D is the mutual diffusion coefficient of the fluids. In simulations of this study, both constant and concentration dependent diffusion coefficients are employed. To account for concentration dependent diffusion coefficient, Vignes' equation (Eq. 4) is used [26]:

$$D(x) = ((D_{BA}^0)^x (D_{AB}^0)^{1-x}) \frac{\partial \ln a_A}{\partial \ln x} \quad (4)$$

In this equation, x is mole fraction of solute (component A), D_{BA}^0 is diffusivity of component B in essentially pure component A, and D_{AB}^0 is diffusivity of component A in essentially pure component B. The last term in Eq.5 is the activity correction factor which assumed to be equal to 1 following the results of [27] at intermediate times of diffusion. A quarter power mixing rule for viscosity (Eq.5) is adopted from [28] and implemented in the simulations to estimate the mixture viscosity-concentration behavior:

$$\mu(x) = \left(\mu_1^{-0.25} + \frac{x}{x_{inj}} (\mu_2^{-0.25} - \mu_1^{-0.25}) \right)^{-4} \quad (5)$$

The subscripts 1 and 2 denote displaced (in-place) and displacing (injected) fluids, respectively. x_{inj} is the mole fraction of solute (component A) in the injecting fluid (fluid 2). Table 1 shows the values of parameters used in the simulations. For constant diffusion coefficient a value of 1×10^{-10} m²/s is assumed for D . The values of D_{BA}^0 and D_{AB}^0 are assumed to be 2×10^{-9} and 5×10^{-11} m²/s, respectively. Note that the value for constant diffusion coefficient (1×10^{-10} m²/s) is equal to the average value of $D(x)$ over the range of $x = 0$ to mole fraction of solute in the injecting fluid ($x = x_{inj}$).

Porous Media Model

The pore scale representation of heterogeneous porous media is achieved by two dimensional packings of circular grains. These media are constructed by random packing of circular grains with different diameters randomly taken from a particle size distribution (PSD). The heterogeneity level of these media can be characterized by a coefficient of variations defined as:

$$CV = \frac{S_{d_p}}{\bar{d}_p} \quad (6)$$

In this definition, \bar{d}_p is the average particle (grain) diameter and S_{d_p} is the standard deviation in diameter (mean and standard deviation of PSD, respectively). Figure 1 shows four media with the same average grain diameter and different coefficients of variation along with their corresponding PSDs. As it is shown in this figure, a higher value of CV results in a more heterogeneous medium with more irregular pore space. The properties of these media are shown in Table 2.

The solid-fluid boundary at the grain surface is considered to be no flow/no slip (zero velocity) for flow and no flux for transport equations. The boundary conditions at the top and bottom boundaries are considered to be symmetrical (zero gradient for velocity and concentration). The inlet condition for flow is constant injection velocity while the outlet is constant atmospheric pressure. For transport equation, constant concentration inflow is imposed on the inlet and outlet boundary condition is assumed to be zero gradient.

Theory of Dispersion

As stated before, dispersion is the combined effect of molecular diffusion and convective spreading in porous media due to variations of velocity field arising from complex structure of pore and throats. This phenomenon in porous media at macro-scale and along the direction of flow can be described by a convection-dispersion equation as:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-K_L \nabla c) + \mathbf{u} \cdot \nabla c = 0 \quad (7)$$

In this equation K_L is the longitudinal dispersion coefficient. Depending on the values of flow velocity, molecular diffusion coefficient, and characteristic length of porous medium, different transport regimes may be encountered during miscible flow. These transport regimes can be correlated to a dimensionless Peclet number defined as:

$$N_P = \frac{uL_c}{D} \quad (8)$$

In this definition, u is the characteristic velocity and L_c is the characteristic length. For random packing of grains, the characteristic length is the average grain diameter and the characteristic velocity is considered to be the injection velocity divided by porosity. Therefore, a pore-Peclet number can be defined as:

$$N_P = \frac{v_{inj} \bar{d}_P}{\phi D} \quad (9)$$

Following [29], the longitudinal dispersion coefficient normalized by molecular diffusion coefficient can be correlated to Peclet number as:

$$\frac{K_L}{D} = \frac{1}{F\phi} + \alpha N_P + \beta N_P^\delta + \gamma N_P^2 \quad (10)$$

In this equation, F is formation factor and α , β , δ , and γ are correlation parameters. At very low Peclet numbers (usually $N_P < 0.1$, [15]) the dominant transport mechanism is pure molecular diffusion. However, because of the presence of solid grains in the path of fluid particles, diffusion is restricted compared to the diffusion in a bulk fluid and therefore the normalized dispersion coefficient is smaller than unity and is equal to $1/F\phi$. At higher Peclet numbers, advection is the dominant transport mechanism. If advection is the sole mechanism of transport (mechanical dispersion), normalized dispersion coefficient scale with N_P (second term on the right hand side of Eq.10). If advection is dominant, but still diffusion from the boundary layer near the surface of solids is contributing to the transport, normalized diffusion coefficient scales with N_P^δ (third term on the right hand side of Eq.10), where the power law coefficient δ is usually between 1.1 to 1.3 [15] with a value of 1.2 for unconsolidated bead packs [30]. The last term in Eq.10 accounts for hold-up dispersion which occurs due to both diffusion from

dead end pores and recirculation. Since in our porous media models usually there is no dead end pore, we can assume that there is no hold-up dispersion, so the last term of Eq. 10 is ignored. The magnitude of dispersion coefficient in a simulated miscible displacement can be calculated by matching the numerically obtained effluent concentration profile at the outlet with the analytical semi-infinite solution of convection-dispersion equation [17,19].

RESULTS AND DISCUSSIONS

We performed several numerical simulations to investigate the effect of injection velocity (in terms of N_p), medium pore scale heterogeneity (in terms of CV), and viscosity ratio of displacing and displaced fluids (in terms of log-viscosity ratio, $R = \ln(\mu_1/\mu_2)$) on the magnitude of dispersion coefficient. Two values of 0 and 3 for log-viscosity ratio are considered and simulations are run on the four media of Figure 1 at different pore-Peclet numbers.

Case 1: $R = 0$, Constant D

The values of longitudinal dispersion coefficient normalized by molecular diffusion coefficient are plotted against pore-Peclet number in Figure 2 for the four porous media of Figure 1. A power law equation has been fit on the data at high Peclet numbers to obtain the value of δ . The results show that $\delta \approx 1.2$ which is in agreement with the value of 1.2 for unconsolidated bead packs [30]. Also, it seems that β is increasing as the heterogeneity of medium (CV) is increasing. All of the graphs of Figure 2 are plotted on a single graph in Figure 3. It is evident that the magnitude of longitudinal dispersion coefficient is higher for more heterogeneous media and this effect of heterogeneity is more significant at larger Peclet numbers.

Case 2: $R = 0$, Concentration-Dependent D

To explore how the concentration dependency of mutual diffusion coefficient affects the performance of miscible displacement, several simulations at unit viscosity ratio are run on the four media considered here. Note that the average value of $D(x)$ in Eq.5 over the concentration range of $x = 0$ to mole fraction of solute in the injecting fluid ($x = x_{inj}$) is equal to the constant diffusion coefficient (1×10^{-10} m²/s) assumed in previous case. The reason is to make the results of case 1 and 2 comparable to each other. Also this value of average diffusion coefficient is used in definition of pore-Peclet number in Figure 4. This figure shows how dispersion coefficient is changing with N_p . The results show that the values of dispersion coefficient and the power low trend line are comparable to that of case 1 (Figure 2). It implies that using an appropriate average value for diffusion coefficient can sufficiently account for the concentration dependency of diffusion coefficient.

Case 3: $R = 3$

Because the results of previous section showed that using an average value of 1×10^{-10} m²/s for diffusion coefficient can predict the same results as using Eq.5 and

corresponding values of D_{BA}^0 and D_{AB}^0 from Table 1, the simulations of miscible displacement at log-mobility ratio of 3 are just performed for the case of constant diffusion coefficient. Figure 5 shows the results of the simulations. The development of vicious fingering due to unfavorable viscosity contrast enhances the mixing and therefore leads to higher values of longitudinal dispersion coefficient compared to results of Figure 3. Also, at this unfavorable viscosity ratio, the normalized longitudinal dispersion coefficient scales with N_p on a log-log plot at all values of $N_p > 0.1$ (Figure 5).

CONCLUSIONS

In this study, pore scale simulations of miscible displacement in heterogeneous two dimensional packings of grains are conducted to estimate the magnitude of longitudinal dispersion coefficient at different values of flow velocity, medium heterogeneity, and viscosity ratio. The results of simulations at a unit viscosity ratio show that at very low Peclet numbers, diffusion is the dominant mechanism of transport, while at high Peclet numbers, transport is advection dominated and dispersion coefficient scales with Peclet number by a power law equation. The heterogeneity of packings described as the ratio of standard deviation in grain diameter to the mean grain diameter is shown to have an impact on dispersion coefficient: more heterogeneous media have higher dispersion coefficients. Also, as long as we use an appropriate average value for diffusion coefficient, it seems that there is no need to consider the concentration dependency of diffusion coefficient. The results of simulations at a higher viscosity ratio demonstrated that the occurrence of viscous fingering gives rise to enhanced mixing and therefore higher values of dispersion coefficient.

ACKNOWLEDGMENT

The authors gratefully acknowledge the financial support of the FUR program from NSERC, AITF/i-CORE, and the sponsoring companies: Laricina Energy, Athabasca Oil Corporation, Devon Canada, Foundation CMG, Husky Energy, Brion Energy, Canadian Natural, Maersk Oil, Suncor Energy, and the Schulich School of Engineering, University of Calgary.

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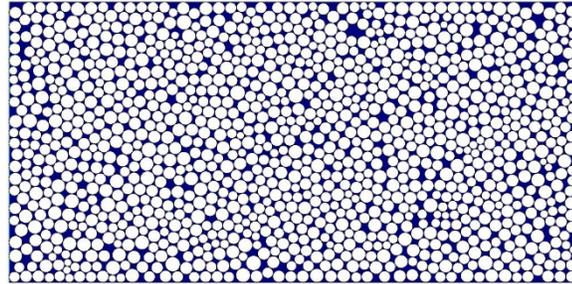
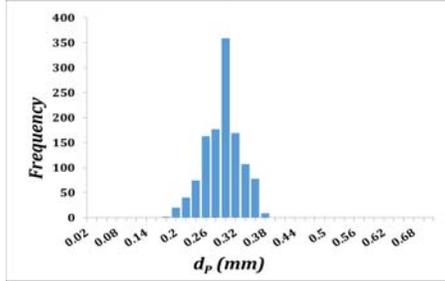
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Table 1. Parameters used in the simulations

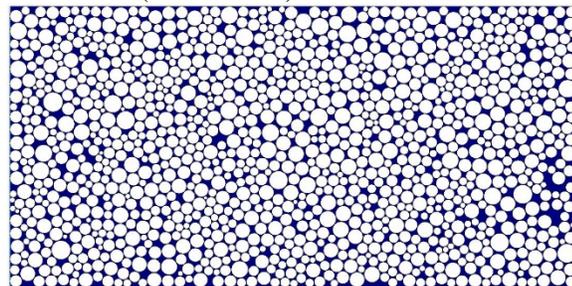
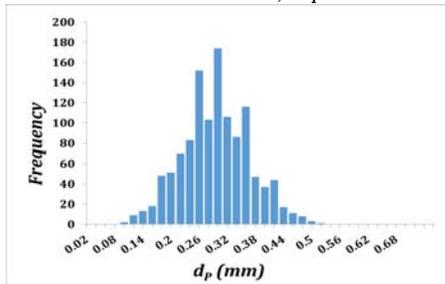
Parameter name	Value
$\rho_A = \rho_B = \rho$	1000 kg/m ³
c_{inj}	1 k-mole/m ³
M_A	100 kg/k-mole
M_B	500 kg/k-mole
x_{inj}	0.357
μ_1	1 and 20 cp
μ_2	1 cp
D (when assumed to be constant)	1×10^{-10} m ² /s
D_{BA}^0	2×10^{-9} m ² /s
D_{AB}^0	5×10^{-11} m ² /s

Table 2. Patterns used in the simulations of this study and their properties

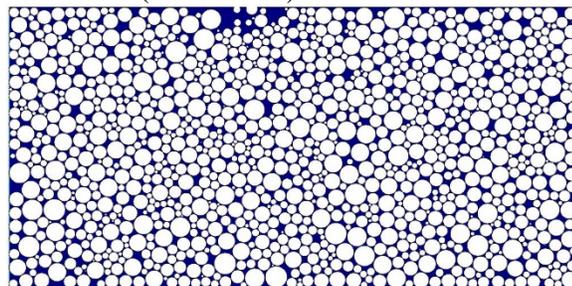
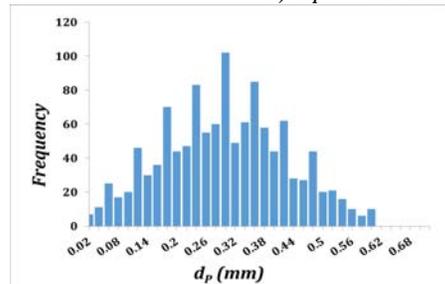
Name	$\overline{d_p}$ (mm)	CV	Number of Particles	Length (L) (mm)	Width (W) (mm)	Porosity	Permeability (Darcy)
C1	0.3	0.13	1200	13.87	6.93	0.240	1.729
C2	0.3	0.25	1200	14.22	7.11	0.235	2.039
C3	0.3	0.44	1200	15.13	7.56	0.227	2.650
C4	0.3	0.53	1200	15.85	7.92	0.253	3.342



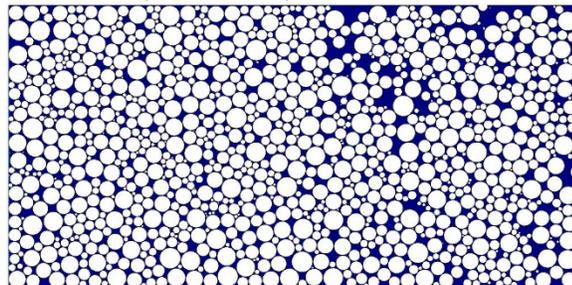
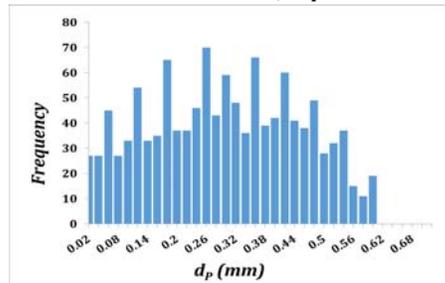
a) $\overline{d_p} = 0.3 \text{ mm}$, $CV = 0.13$ (medium C1)



b) $\overline{d_p} = 0.3 \text{ mm}$, $CV = 0.25$ (medium C2)



c) $\overline{d_p} = 0.3 \text{ mm}$, $CV = 0.44$ (medium C3)



$$d) \overline{d_p} = 0.3 \text{ mm} , CV = 0.53 \text{ (medium C4)}$$

Figure 1. Sample media with the same $\overline{d_p}$ and different CV along with their corresponding PSDs

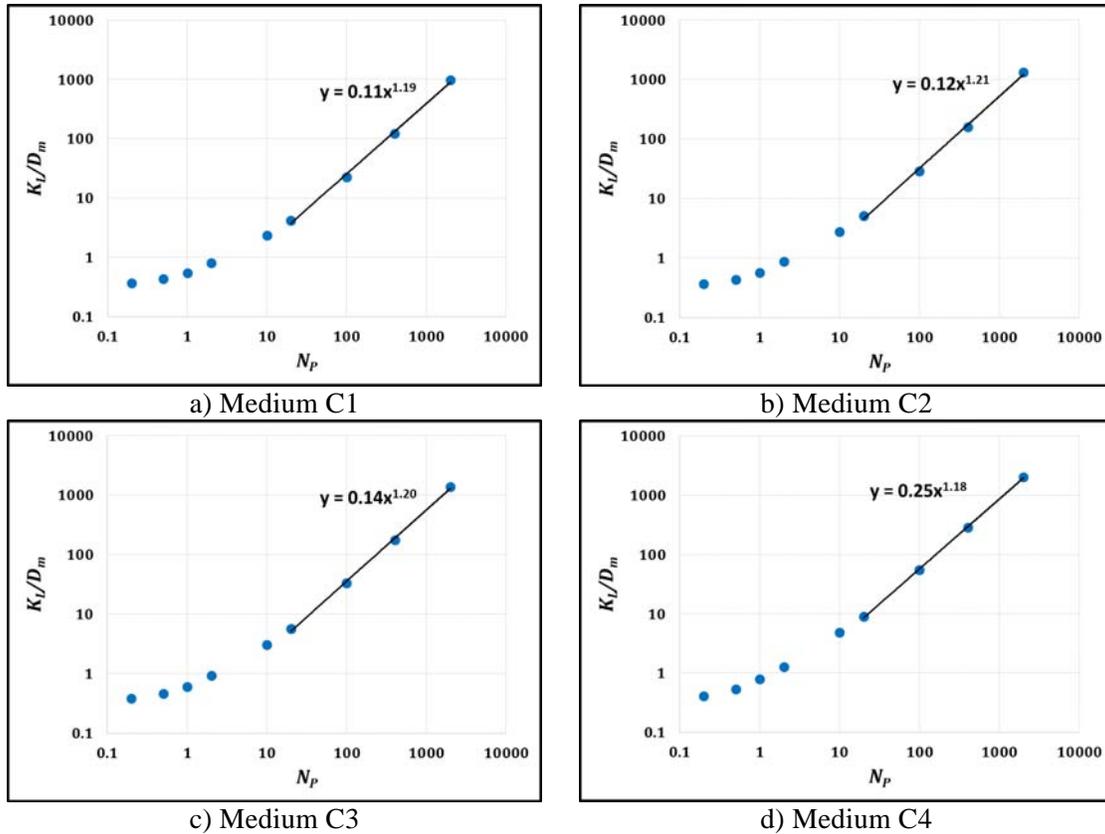


Figure 2. Variation of normalized longitudinal dispersion coefficient with pore-Peclet number at unit viscosity ratio ($R = 0$) and constant diffusion coefficient of $1 \times 10^{-10} \text{ m}^2/\text{s}$

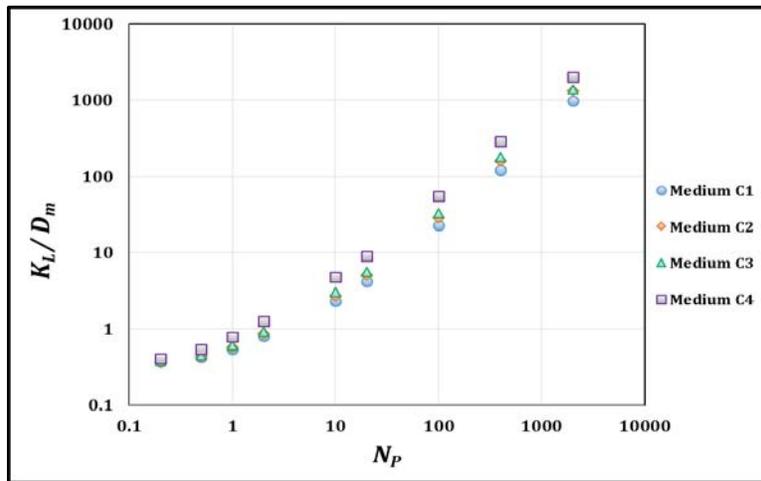


Figure 3. Effect of medium heterogeneity on longitudinal dispersion coefficient at unit viscosity ratio ($R = 0$) and constant diffusion coefficient of $1 \times 10^{-10} \text{ m}^2/\text{s}$

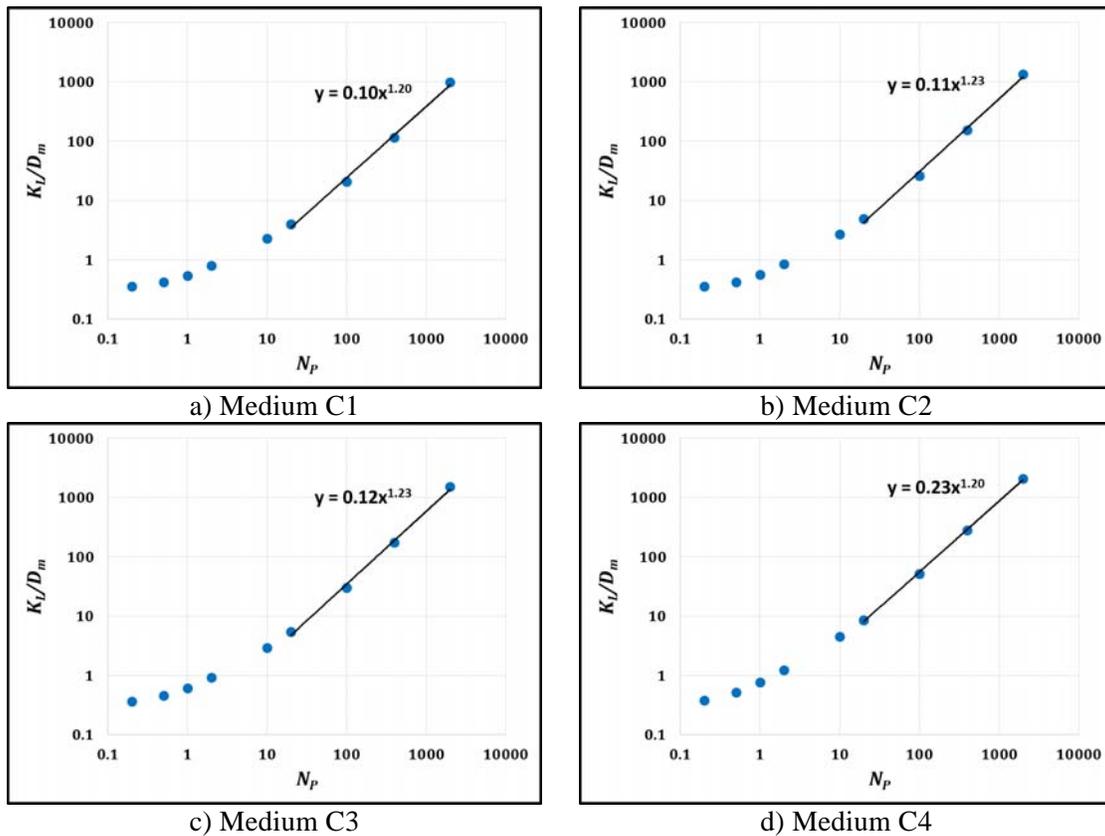


Figure 4. Variation of normalized longitudinal dispersion coefficient with pore-Peclet number at unit viscosity ratio ($R = 0$) and concentration-dependent diffusion coefficient

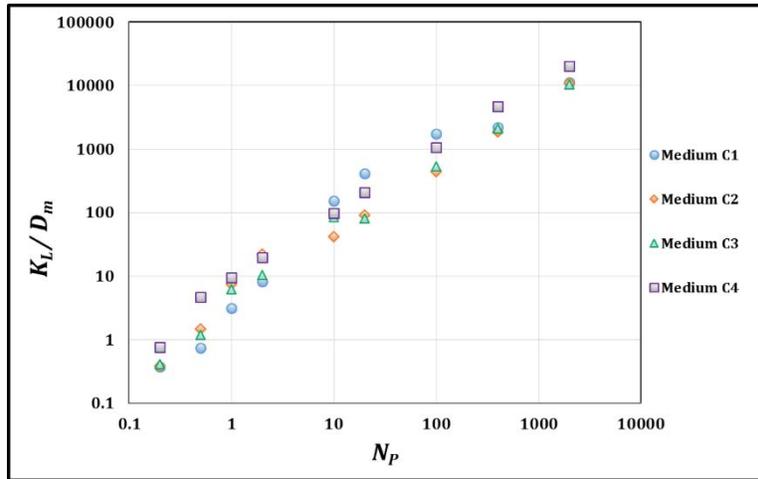


Figure 5. Variation of normalized longitudinal dispersion coefficient with pore-Peclet number at unfavorable viscosity ratio ($R = 3$) and constant diffusion coefficient of $1 \times 10^{-10} \text{ m}^2/\text{s}$