Available online at www.sciencedirect.com

ScienceDirect

Advances in Water Resources 30 (2007) 199–213

Advances in Water Resources

www.elsevier.com/locate/advwatres

Quantification of longitudinal dispersion by upscaling Brownian motion of tracer displacement in a 3D pore-scale network model

R.C. Acharya [a,*], M.I.J. van Dijke [b], K.S. Sorbie [b], S.E.A.T.M. Van der Zee [a], A. Leijnse [a]

[a] Department of Environmental Sciences, Wageningen University, P.O. Box 47, 6700 AA Wageningen, The Netherlands
[b] Institute of Petroleum Engineering, Heriot–Watt University, Riccarton Campus, Edinburgh EH14 4AS, UK

Received 24 August 2004; received in revised form 3 April 2005; accepted 12 April 2005
Available online 9 March 2006

Abstract

We present a 3D network model with particle tracking to upscale 3D Brownian motion of non-reactive tracer particles subjected to a velocity field in the network bonds, representing both local diffusion and convection. At the intersections of the bonds (nodes) various jump conditions are implemented. Within the bonds, two different velocity profiles are used. At the network scale the longitudinal dispersion of the particles is quantified through the coefficient D_L, for which we evaluate a number of methods already known in the literature. Additionally, we introduce a new method for derivation of D_L based on the first-arrival times distribution (FTD). To validate our particle tracking method, we simulate Taylor's classical experiments in a single tube. Subsequently, we carry out network simulations for a wide range of the characteristic Péclet number Pe_ℓ to assess the various methods for obtaining D_L. Using the new method, additional simulations have been carried out to evaluate the choice of nodal jump conditions and velocity profile, in combination with varying network heterogeneity. In general, we conclude that the presented network model with particle tracking is a robust tool to obtain the macroscopic longitudinal dispersion coefficient. The new method to determine D_L from the FTD statistics works for the full range of Pe_ℓ, provided that for large Pe_ℓ a sufficiently large number of particles is used. Nodal jump conditions should include molecular diffusion and allow jumps in the upstream direction, and a parabolic velocity profile in the tubes must be implemented. Then, good agreement with experimental evidence is found for the full range of Pe_ℓ, including increased D_L for increased porous medium heterogeneity.

Keywords: Dispersion; Transport; Pore network; Brownian motion; Particle tracking; Nodal jump condition; Moment methods; Pore to core

1. Introduction

Dispersion in porous media is of interest in many fields, such as chemical, petroleum, civil and environmental engineering [1]. It plays an important role in the accuracy of predictions during reactive and non-reactive transport in groundwater systems (porous media). In porous media, dispersion is caused by two processes: Brownian motion of solute molecules, or *molecular diffusion* and the velocity differences among solute-carrying solvent-streamlines, which is referred to as *mechanical* dispersion. The interplay of these two phenomena leads to the *hydrodynamic* dispersion [2].

Because of its key role in the theory of mass transport, the dispersion process has been studied for a considerable time [3–6]. In general, two methodologies (models) have been devised to describe dispersion viz the deterministic (e.g., [7]), and probabilistic or statistical approaches (e.g., [8–11]). The mixing cell model is an example of the first, whereas the particle tracking approach in combination with the method of moments serves as an example of the second approach. Dispersion is a scale- and velocity field-dependent phenomenon [12]. At the continuum scale, Bear [7] showed that dispersion takes the form of a second order

---

[*] Corresponding author. Fax: +31 317 483766.

E-mail addresses: hypon@uiuc.edu (R.C. Acharya), Rink.VanDijke@pet.hw.ac.uk (M.I.J. van Dijke), ken.sorbie@pet.hw.ac.uk (K.S. Sorbie), sjoerd.vanderzee@wur.nl (S.E.A.T.M. Van der Zee), toon.leijnse@wur.nl (A. Leijnse).

0309-1708/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2005.04.017

Nomenclature

$\langle \cdot \rangle$	ensemble average quantity
C, $\widetilde{C}$	concentration [M L^{-3}] and dimensionless concentration
D, D_{L}, D_{T}	dispersion coefficients: effective, longitudinal and Taylor [L^2 T^{-1}]
D_{m}, D_{h}	molecular diffusion coefficient and mechanical dispersion [L^2 T^{-1}]
$f_{i,j}$	advection–diffusion fraction factor of Sorbie–Clifford formulation
$f(\lambda)$	intra-pore velocity function
H	Heaviside integral
i, j	the indices of nodes and bonds
k_{ax}	Taylor's coefficient for cross-section shape (e.g., 1/48)
L, ℓ	length of the pore-network and bond length [L]
Pe_{L}	pore network (Column) Péclet number vL/D_{L}
$p(i,j)$	transition probability density function
Pe_{b}, Pe_{T}	bond Péclet and Taylor's Péclet numbers [–]
Pe_{ref}	a reference (conditional) threshold Bond Péclet number [–]
Pe_{ℓ}	characteristic Péclet number $v\ell/D_{\mathrm{m}}$ [–]
$q_{i,j}$, Q	discharge, respectively, through bonds and pore-network [L^3 T^{-1}]
R, $\widetilde{R}$	radius [L] and aspect ratio (R/ℓ) of bonds (Taylor's tubes)
$\Delta\mathbf{r}$	radius vector of Brownian sphere [L]
Re	Reynolds number (dimensionless)
Sc	Schmidt number (dimensionless)
t, Δt	time and time step of iteration [T]
$\widetilde{T}$	dimensionless time on network scale (vt/L)
U, u	actual and mean velocity in the Taylor's tubes [L T^{-1}]
v	mean intrinsic velocity along the principle flow direction in the pore network [L T^{-1}]
W_Y, W_Z	transversal horizontal and vertical lengths of the network ($\perp X$) [L]
x, y	local reference system, $x \in [0, \ell]$ along the axial direction of fluid flow [L]
X, Y, Z	global (network scale) reference system [L]
β	an exponent parameter
$\phi(\Delta\mathbf{r})$	Green's probability function for Markov's processes
λ	dimensionless local radial coordinate
μ	ensemble average as specified with subscript (e.g., μ_t and μ_X)
ν	kinematic viscosity of fluid [L^2 T^{-1}]
σ^2	second central spatial moment (variance) of positions of particles with respect to a chosen direction (e.g., σ_X^2) [L^2]
τ	dimensionless time on pore-scale (ut/ℓ)
ξ	local axis (x/ℓ) along flow in a capillary [–]
ϖ	a factor in Sorbie–Clifford formulation $(\pi R^2)/\ell$ [L]
φ	polar angle of radius vector in Brownian spherical coordinate system $[0, \pi]$
ψ	deviate of the Green's function [–]
ζ	tortuosity [–]
θ	azimuthal angle of radius vector in Brownian spherical coordinate system $[0, 2\pi]$
T, m, L, b	subscripts indicate Taylor, molecular, Longitudinal and bond
CDE	convection–dispersion equation
(C) FTD	(cumulative) first-arrival times distribution
SPD	spatial position distribution

tensor that depends not only on local variations of velocity field but also on large-scale characteristics of the medium [7,8]. This tensor is used in the convection–dispersion equation (CDE). Alongside theoretical developments in dispersion theory, experimental and numerical works have emerged to determine the dispersion tensor [13,14]. Historical reviews of dispersion research can be found in [7,14–22].

As mentioned above, dispersion originates from variation of velocity at the pore scale (Taylor scale), i.e., within a pore cross-section, as well as from geometrical variation of the length scale of the distribution of pores within a porous medium. A first attempt to average these variations at the pore scale to an effective property at the continuum scale was made by Saffman [23]. Following Fatt [24], Saffman used a pore network model as a tool to include the pore-scale physical phenomena. Since the work of Saffman, 2D network models, in combination with random-walker particle tracking, have often been employed to upscale the pore-scale dispersion coefficient to a network-scale quantity [10,11,14,25–27]. However, so far only qualitative agreement with experimental results has been obtained [10] and a rigorous quantitative upscaling of multi-directional Brownian walker (3D motion of material points) from the Brownian sphere to the 3D pore network has not yet been presented.

One of the main reasons that has prevented such rigorous upscaling lies in the uncertainty of the mixing conditions and transition probabilities at the intersection of pores (nodes) in a network model [26–29]. The simplest assumption is to take the transition probability at a node proportional to the flow rates in the neighboring bonds [5]. However, this method excludes the effect of molecular diffusion at the nodes. A more sophisticated approach consists of constructing a pattern of streamlines from inflowing to outflowing bonds at a node, such that the intra-pore particle tracking can be continued from pore to pore [9,29]. This method has successfully been constructed in 2D, but