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Uncertainty and sensitivity analysis of filtration models for non-Fickian transport and hyperexponential deposition

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ABSTRACT

Uncertainty and sensitivity analyses are carried out to investigate the predictive accuracy of the filtration models for describing non-Fickian transport and hyperexponential deposition. Five different modeling approaches, involving the elliptic equation with different types of distributed filtration coefficients and the CTRW equation expressed in Laplace space, are selected to simulate eight experiments. These experiments involve both porous media and colloid–medium interactions of different heterogeneity degrees. The uncertainty of elliptic equation predictions with distributed filtration coefficients is larger than that with a single filtration coefficient. The uncertainties of model predictions from the elliptic equation and CTRW equation in Laplace space are minimal for solute transport. Higher uncertainties of parameter estimation and model outputs are observed in the cases with the porous media and the colloid–medium interactions of higher heterogeneity. The parameters for the distribution of filtration coefficients could not be uniquely identified due to strong correlations. In the cases of heterogeneous colloid–medium interactions where hyper-exponential deposition is observed, the distribution of filtration coefficients could not be accurately determined by the effluent concentration profile alone. Measurements of deposition are necessary. The effluent concentrations around the breakthrough and around the end of colloid injection are more sensitive to dispersion coefficients than filtration coefficients, while deposition is more sensitive to filtration coefficients. Based on the insights and information provided by the uncertainty and sensitivity analysis of the filtration models, the following are concluded: (i) it is possible to improve the parameter estimation accuracy by doing more measurements at sensitivity-focused moments. (ii) the elliptic equation with distributed filtration coefficients is more accurate at modelling colloids filtration where heterogeneity of particle-medium interactions is dominant, and (iii) Both the elliptic equation and the CTRW equation are accurate at modeling transport in ground water or other systems where the median heterogeneity is dominant.

1. Introduction

Modeling suspension or colloid flow in porous media is of great importance to a large variety of applications, e.g. deep bed filtration, membrane filtration, drilling mud filtration, bacteria and viruses spreading in underground water and others [1–3]. There is a considerable and ongoing effort aimed at understanding the transport and the deposition of suspended particles in porous media. Especially, non-Fickian transport and non-exponential deposition of particles, such as hyperexponential deposition profiles or even non-monotonic deposition profiles, attract significant interest [4–12].

Non-Fickian behavior of the suspensions in porous media may be caused by the physical heterogeneity of porous media [4–7,13–17]. It has been indicated by a number of works [4,6,7,13–15,18,19] that non-Fickian transport of a solute or a suspension may be modeled more accurately by approaches based on the continuous time random walk (CTRW) theory compared to the classical advection dispersion equation (ADE). The first CTRW model for colloidal transport in porous media was studied in Ref. [15].

A macroscopic elliptic equation for non-Fickian transport in porous media in the framework of CTRW [13,18,19] was developed by Shapiro and Bedrikovetsky. The equation can be applied to describe either the transport of macroscopic particles or that of the solute in porous media. The elliptic equation and the distribution of filtration coefficients can be integrated as an integral model to describe non-Fickian transport of polydisperse suspension in heterogeneous porous media [7,13]. Recently, the approach has been tested to compare with experimental observations in different types of porous media, such as packed glass beads, packed sand and artificially heterogeneous porous media [7]. It was observed that in highly heterogeneous porous media where the non-Fickian trans-

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Nomenclature

c_i	number of suspended particles per unit pore volume (m^{-3})
C_i	dimensionless suspended particle concentration
s_i	number of retained particles per unit volume of porous media (m^{-3})
S_i	dimensionless retained particle concentration
t	time (s)
T	dimensionless time (pore volume)
x	x coordinate in space
X	dimensionless x
N_c	number of retained particles per gram of porous media
N_t	number of total injected particles
v	interstitial velocity of particles (m/s)
V	dimensionless interstitial velocity of particles
a	Correction coefficient to ensure the unity of a discrete distribution
b	Power for the power-law distribution of Λ
v_ψ	velocity of CTRW interpretations
D_ψ	dispersion coefficient of CTRW interpretations (m^2/s)
D_x	coefficient of spatial dispersion (m^2/s)
D_t	coefficient of temporal dispersion (s)
R_x	dimensionless longitudinal dispersivity
R_t	dimensionless temporal dispersivity
M	memory function in CTRW theory
$\bar{\psi}$	core expression in the memory function of CTRW
β	parameter of the truncated power law model for CTRW
$\bar{t}$	characteristic time of porous media (s)
t_1	lower limit of the truncated power law model for CTRW (s)
t_2	upper limit of the truncated power law model for CTRW (s)
u	Laplace variable
p	probability density function
t_0	particle injection duration (s)
T_0	particle injection duration (pore volume)
c_0	influent concentration
μ	mean value
σ	standard deviation
λ	filtration coefficient (s^{-1})
Λ	dimensionless filtration coefficient
$\Lambda_{\min}$	lower limit of the distribution of filtration coefficients
$\Lambda_{\max}$	upper limit of the distribution of filtration coefficients
ξ	total injection time is ξ times the particle injection duration
φ	porosity of the porous media
ρ_b	bulk density of the dry porous media
δ^{msqr}	sensitivity measure
C^s	scaled concentration with respect to Monte Carlo simulations
S^s	scaled deposition with respect to Monte Carlo simulations
$S_{nd,jl}$	non-dimensional sensitivity of jth parameter at ith data point
θ	any parameter
y	model output of C or S
y_{reg}	model output based on linear regression of Monte Carlo simulations
N	number of experimental data/calculation points
n	number of measured data points
P	number of parameters for estimation
η	standardized regression coefficients
i	index of suspended particle species
j	index of parameters
k	index of Monte Carlo simulations
l	index of measured data points

port is observed the elliptic equation excels the ADE and predicts hyperexponential deposition profiles.

Besides the median heterogeneity leading to the non-Fickian breakthrough curves, the heterogeneity of colloid–medium interactions or particle population gives rise to hyperexponential deposition profiles. The commonly reported hyperexponential deposition has been attributed to the heterogeneity of the surface charge and energy minima [9,10,20,21] or to the enhanced retention at low-velocity zones of pore space (physical straining) [22–24]. Based on the described mechanisms, the authors developed various models which produce hyperexponential deposition. In Refs. [7,9,10,21], distributions of filtration coefficients were applied to reflect the heterogeneity of particle population and particle–pore interactions. In Refs. [24,25], dual-permeability models were developed to take into account the high-velocity zones and low-velocity zones of pore space.

The temporal dispersion term and the distribution of filtration coefficients are two advances compared to the traditional approach. To the best of our knowledge, their properties can only be estimated by fitting breakthrough curves and deposition profiles to the experimental data [7,9,10]. Whether the additional parameters can be uniquely identified or how large is the uncertainty of parameter estimation remains unknown.

Generally, there are various sources of uncertainty of the model outputs, such as the input uncertainty reflecting the lack of knowledge or accuracy of the model inputs, and the structural uncertainty related to the mathematical interpretation of the model [26]. From the uncertainty analysis, a probability distribution of model outputs can be obtained, including the mean value, the variances and the quantiles [27–29].

The uncertainties of the integral elliptic model may come from the following sources. (i) The approximation of particle velocity by the average pore water velocity; it has been observed that the particles of different sizes may travel faster or slower that the carrying fluid in porous media [30]. (ii) Estimation of dispersion coefficients by fitting to experiments; for highly heterogeneous porous media the observed breakthrough curves are more dispersed and contain more scattered points [7,31]. (iii) Lack of understanding heterogeneity of particle population. The heterogeneity of particle population may be reflected by distributions of particle properties [7,10,21]. The relation between the distribution types and the heterogeneity has not been fully understood, yet.

On the other hand, the sensitivity analysis aims at quantifying the individual contribution from each parameter's uncertainty to the uncertainty of outputs. Correlations between parameters may also be inferred from sensitivity analysis. It is a frequent routine and recommended to perform the uncertainty and sensitivity analysis in tandem [27,32–35].

In this work, uncertainty and sensitivity analyses are carried out to investigate the predictive accuracy of the filtration models for non-Fickian transport and hyperexponential deposition. Five different modeling approaches, involving the elliptic equation with different types of distributed filtration coefficients and the CTRW equation expressed in Laplace space, are selected to simulate a