Advances in Water Resources 68 (2014) 62–73

Contents lists available at ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

Mathematical modeling of colloid and virus cotransport in porous media: Application to experimental data

Vasileios E. Katzourakis [a], Constantinos V. Chrysikopoulos [b,*]

[a] Environmental Engineering Laboratory, Civil Engineering Department, University of Patras, Patras 26500, Greece
[b] School of Environmental Engineering, Technical University of Crete, Chania 73100, Greece

ARTICLE INFO

Article history:
Received 23 August 2013
Received in revised form 24 December 2013
Accepted 3 March 2014
Available online 21 March 2014

Keywords:
Viruses
Colloids
Cotransport
Mathematical modeling
Porous media

ABSTRACT

A conceptual mathematical model was developed to describe the simultaneous transport (cotransport) of viruses and colloids in three-dimensional, water saturated, homogeneous porous media with uniform flow. The model accounts for the migration of individual virus and colloid particles as well as viruses attached onto colloids. Viruses can be suspended in the aqueous phase, attached onto suspended colloids and the solid matrix, and attached onto colloids previously attached on the solid matrix. Colloids can be suspended in the aqueous phase or attached on the solid matrix. Viruses in all four phases (suspended in the aqueous phase, attached onto suspended colloid particles, attached on the solid matrix, and attached onto colloids previously attached on the solid matrix) may undergo inactivation with different inactivation coefficients. The governing coupled partial differential equations were solved numerically using finite difference methods, which were implemented explicitly or implicitly so that both stability and speed factors were satisfied. Furthermore, the experimental data collected by Syngouna and Chrysikopoulos [1] were satisfactorily fitted by the newly developed cotransport model.

1. Introduction

Mathematical modeling of contaminant, colloid and biocolloid (virus, protozoa, and bacteria) transport in subsurface formations has captured the attention of several scientists and environmental engineers, because of the increased public concern and attention paid to the disposal, movement and fate of contaminants in natural systems. Groundwater contaminated with pathogenic microorganisms has severe consequences to public health throughout the world, but particularly in small communities and developing countries, where untreated groundwater is often consumed [2]. Although waterborne diseases can be controlled, outbreaks continue to exist [3]. The majority of the waterborne diseases reported in the United States during the time period 1971–2006 were associated with cases of groundwater contamination [4]. Therefore, understanding the transport mechanisms that control biocolloid migration through subsurface formations is essential for the protection of public health.

Numerous experimental and theoretical studies have focused on factors that govern colloid and biocolloid transport in fractured and porous media [5–21]. Of particular importance is the presence of colloids suspended in the aqueous phase. It should be noted that colloids are small particles with size in the range 1 nm to 10 μm [22] that occur naturally in practically every aquatic system due to precipitation of supersaturated phases, mobilization of existing colloidal phases, well drilling, leaching from the vadose zone, and dissolution of inorganic cementing agents that bind colloid-size materials to solid surfaces [23–26]. Colloids remain suspended in water for long time because they have low sedimentation rate, and undergo random Brownian motion while carrying surface electric charge. Many pollutants, including biocolloids, in aqueous media are readily adsorbed/attached onto colloidal particles, which often act as carriers. Several experimental and theoretical studies have shown that, depending on the physicochemical conditions of the fractured and porous media, colloids can either enhance or hinder the transport of organic and inorganic pollutants [27–45].

Several research groups have developed analytical and numerical mathematical models to describe and predict colloid and biocolloid transport in fractured and porous media [46–56]. Furthermore, a few mathematical models have been developed to describe facilitated contaminant and biocolloid transport in fractured and porous media [28,57–61].

The objective of the present study is to (a) improve the one-dimensional mathematical model for colloid-facilitated bacteria transport developed by Vasiliadou and Chrysikopoulos [61] for colloid-facilitated virus transport in three-dimensional, water saturated, homogeneous porous media with uniform flow, (b) provide an efficient numerical solution to the newly developed virus–colloid cotransport model, and (c) apply the numerical model to

* Corresponding author. Tel.: +30 28210 37797; fax: +30 28210 37847.
E-mail address: cvc@enveng.tuc.gr (C.V. Chrysikopoulos).

http://dx.doi.org/10.1016/j.advwatres.2014.03.001
0309-1708/

Nomenclature

C_i	concentration of suspended species i, M/L^3
C_i^*	concentration of species i attached onto the solid matrix, M_i/M_s
C_c	concentration of suspended colloids, M_c/L^3
C_c^*	concentration of colloids attached onto the solid matrix, M_c/M_s
C_v	concentration of suspended viruses, M_v/L^3
C_v^*	concentration of viruses attached onto the solid matrix, M_v/M_s
C_{vc}	concentration of viruses attached onto suspended colloid particles, M_v/M_c
C_{vc}^*	concentration of virus–colloid particles attached onto the solid matrix, M_v/M_c
$C_c^{*(r)}$	concentration of colloids reversibly attached onto the solid matrix, M_c/M_s
$C_c^{*(i)}$	concentration of colloids irreversibly attached onto the solid matrix, M_c/M_s
C_{oi}	initial concentration of suspended species i, M_i/L^3
D_{xi}	longitudinal hydrodynamic dispersion coefficient of species i, L^2/t
D_{yi}	lateral hydrodynamic dispersion coefficient of species i, L^2/t
D_{zi}	vertical hydrodynamic dispersion coefficient of species i, L^2/t
$\mathcal{D}_{ei}$	effective diffusion coefficient of species i, L^2/t
$\mathcal{D}_{iw}$	molecular diffusion coefficient of species i in fluid w (water), L^2/t
F_c	general form of colloids source configuration, M_c/L^3t
F_v	general form of viruses source configuration, M_v/L^3t
i	species c = colloid, v = virus, vc = virus–colloid
L_x	length of porous medium (packed column), L
L_y	width of porous medium, L
L_z	height of porous medium, L
L	length, L
M_c	mass of colloids, M_c
M_s	mass of the solid matrix, M_s
M_v	mass of viruses, M_v
n_x	number of discretization unit cells in the x-direction, (–)
Q	flow rate, L^3/t
$r_{c-c^{*(i)}}$	rate coefficient of irreversible colloid attachment onto the sold matrix, $1/t$
$r_{c^{*(r)}-c}$	rate coefficient of reversible colloid detachment from the solid matrix, $1/t$
$r_{c-c^{*(r)}}$	rate coefficient of reversible colloid attachment onto the sold matrix, $1/t$
r_{v-v^*}	rate coefficient of virus attachment onto the solid matrix, $1/t$
r_{v^*-v}	rate coefficient of virus detachment from the solid matrix, $1/t$
r_{v-vc}	rate coefficient of virus attachment onto suspended colloid particles, L^3/M_ct
r_{vc-v}	rate coefficient of virus detachment from suspended colloid particles, $1/t$
$r_{v-v^*c^*}$	rate coefficient of virus attachment onto colloid particles already attached ontothe solid matrix, L^3/M_ct
$r_{vc-v^*c^*}$	rate coefficient of virus–colloid particle attachment onto the solid matrix, $1/t$
$r_{v^*c^*-v}$	rate coefficient of virus detachment from colloid particles attached onto the solid matrix, $1/t$
$r_{v^*c^*-vc}$	rate coefficient of virus–colloid particle detachment from the solid matrix, $1/t$
t	time, t
t_p	injection time period, t
U	interstitial velocity, L/t
X	spatial coordinate in the longitudinal direction, L
Y	spatial coordinate in the lateral direction, L
Z	spatial coordinate in the vertical direction, L

Greek letters

α_L	longitudinal dispersivity, L
α_{T_y}	transverse (lateral) dispersivity, L
α_{T_z}	transverse (vertical) dispersivity, L
$\delta(x)$	Dirac delta function, $1/L$
θ	porosity of the column material, (L^3 voids)/(L^3 solid matrix)
λ_v	decay rate of viruses suspended in the liquid phase, $1/t$
λ_v^*	decay rate of viruses sorbed or attached onto the solid matrix, $1/t$
λ_{vc}	decay rate of virus–colloid complexes suspended in the liquid phase, $1/t$
λ_{vc}^*	decay rate of virus–colloid complexes sorbed or attached onto the solid matrix, $1/t$
Λ_{v-vc}	mass accumulation rate due to attachment of suspended viruses onto suspended colloid particles, M_v/L^3t
$\Lambda_{v-v^*c^*}$	mass accumulation rate due to attachment of suspended viruses onto colloid particles already attached onto the solid matrix, M_v/L^3t
Λ_{vc-v}	mass accumulation rate due to virus detachment from suspended colloid particles, M_v/L^3t
$\Lambda_{v^*c^*-v}$	mass accumulation rate due to virus detachment from colloid particles attached onto the solid matrix, M_v/L^3t
$\Lambda_{vc-v^*c^*}$	mass accumulation rate due to attachment of suspended virus–colloid particles onto the solid matrix, M_v/L^3t
$\Lambda_{v^*c^*-vc}$	mass accumulation rate due to detachment of virus–colloid particles from the solid matrix, M_v/L^3t
ρ_b	bulk density of the solid matrix, M_s/L^3
τ^*	tortuosity, (–)

the experimental data for bacteriophage (MS2, ΦX174) and clay (kaolinite, montmorillonite) cotransport, published by Syngouna and Chrysikopoulos [1]. To our knowledge no other three-dimensional colloid and virus cotransport model together with its efficient and robust numerical solution has neither been presented in the literature nor has been employed to available experimental data before.

2. Model development

The proposed colloid facilitated virus transport model assumes that the colloids partition between the aqueous phase and the solid matrix, while viruses may attach onto colloidal particles in the aqueous phase, onto the solid matrix, and onto colloids previously attached onto the solid matrix. Consequently, colloid particles can be suspended in the aqueous phase C_c [M_c/L^3], or attached onto the solid matrix C_c^* [M_c/M_s]. Viruses can be suspended in the aqueous phase C_v [M_v/L^3], directly attached onto the solid matrix C_v^* [M_v/M_s], attached onto suspended colloid particles (virus–colloid particles) C_{vc} [M_v/M_c], and attached onto colloid particles already attached onto the solid matrix (or equivalently virus–colloid particles attached onto the solid matrix) C_{vc}^* [M_v/M_c]. A schematic illustration of the various types of concentrations considered in the present mathematical model is given in Fig. 1. To simplify the notation, the various masses are indicated as follows: M_c is the mass of colloids, M_v is the mass of viruses, and M_s is the mass of the solid matrix. Also, the subscripts c, v, and vc represent colloid, virus and virus–colloid, respectively.