Numerical modeling of colloid facilitated virus transport in porus media

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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 onto 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 by employing finite difference methods, which were implemented explicitly or implicitly so that both stability and accuracy factors were satisfied. Furthermore, pertinent experimental data published by Synguna and Chrysikopoulos (2013) were satisfactorily fitted by the newly developed cotransport model.

Model development

The colloid facilitated virus transport model assumes that the colloids partition between the aqueous phase and the solid matrix, while viruses attach onto colloid particles and the solid matrix. Consequently, colloid particles can be suspended in the aqueous phase, or attached onto the solid matrix. Viruses can be suspended in the aqueous phase, directly attached onto the solid matrix, attached onto suspended colloid particles (virus-colloid particles), and attached onto colloid particles that are already attached onto the solid matrix (or equivalently virus-colloid particles attached onto the solid matrix). 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.

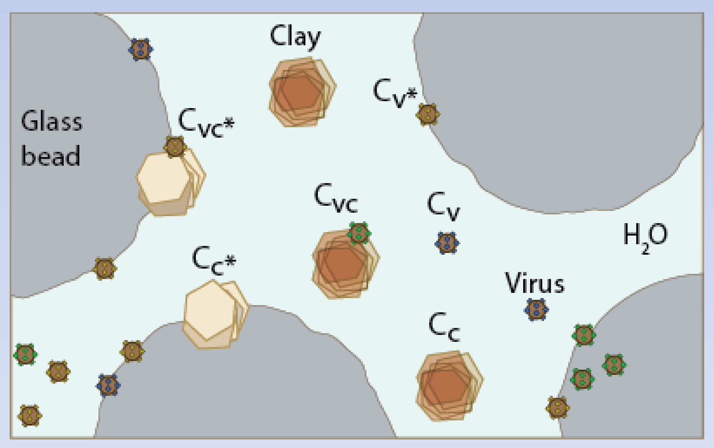

Figure 1: Schematic illustration of the various concentrations accounted for in the cotransport mathematical model.

- C_c colloid particles suspended in the aqueous phase $[M_c/L^3]$
- C_c^* colloid particles attached onto the solid matrix:
  - a) Due to adsorption $C_c^{*(r)}$ $[M_c/M_s]$ (r=reversible)
  - b) Due to deposition $C_c^{*(i)}$ $[M_c/M_s]$ (i= irreversible)
- C_v Viruses suspended in the aqueous phase $[M_v/L^3]$
- C_v^* Viruses Directly attached onto the solid matrix $[M_v/M_s]$
- C_{vc} Viruses attached onto suspended colloid particles (virus-colloid particles) $[M_v/M_c]$,
- C_{vc}^* Viruses attached onto colloid particles that are already attached onto the solid matrix (or equivalently virus-colloid particles attached onto the solid matrix) $[M_v/M_c]$

Mathematical Model

Governing partial differential equations

3-D Colloid transport equation
(Sim and Chrysikopoulos, 1998, 1999; Fabrice Compere et al., 2001)

$$\frac{\partial C_c(t,x,y,z)}{\partial t}+\frac{\rho_b}{\theta}\left(\frac{\partial C_c^{*(r)}(t,x,y,z)}{\partial t}+\frac{\partial C_c^{*(i)}(t,x,y,z)}{\partial t}\right)-D_{xc}\frac{\partial^2 C_c(t,x,y,z)}{\partial x^2}-D_{yc}\frac{\partial^2 C_c(t,x,y,z)}{\partial y^2}-D_{zc}\frac{\partial^2 C_c(t,x,y,z)}{\partial z^2}+U\frac{\partial C_c(t,x,y,z)}{\partial x}=F_c$$

Reversible colloid adsorption 1st order equation
(Sim and Chrysikopoulos, 1998)

$$\frac{\rho_b}{\theta}\frac{\partial C_c^{*(r)}(t,x,y,z)}{\partial t}=r_{c\text{-}c^{*(r)}}C_c(t,x,y,z)-r_{c^{*(r)}\text{-}c}\frac{\rho_b}{\theta}C_c^{*(i)}(t,x,y,z)$$

Irreversible colloid adsorption 1st order equation
(Fabrice Compere et al., 2001)

$$\frac{\rho_b}{\theta}\frac{\partial C_c^{*(i)}(t,x,y,z)}{\partial t}=r_{c\text{-}c^{*(i)}}C_c(t,x,y,z)$$

Adsorbed colloid-virus complex mass accumulation rate
(Bekhit et al., 2009)

$$\frac{d}{dt}(C_cC_{vc})=r_{v-vc}(C_{vc_{eq}}-C_{vc})^2C_c-r_{vc-v}(C_cC_{vc})+\frac{\rho_b}{\theta}r_{v^*c^*-vc}(C_c^*C_{vc}^*)-r_{vc-v^*c^*}(C_cC_{vc})-\lambda_{vc}C_cC_{vc}$$

Suspended colloid-virus complex mass accumulation rate
(Bekhit et al., 2009)

$$\frac{\rho_b}{\theta}\frac{d}{dt}(C_c^*C_{vc}^*)=\frac{\rho_b}{\theta}r_{v-v^*c^*}(C^*_{vc_{eq}}-C^*_{vc})^2C_c^*-\frac{\rho_b}{\theta}r_{v^*c^*-v}(C_c^*C_{vc}^*)+r_{vc-v^*c^*}(C_cC_{vc})-\frac{\rho_b}{\theta}r_{v^*c^*-vc}(C_c^*C_{vc}^*)-\lambda_{vc}^*\frac{\rho_b}{\theta}C_c^*C_{vc}^*$$

Colloid facilitated virus transport equation
(Vasiliadou and Chrysikopoulos, 2011)

$$\frac{\partial}{\partial t}\left(C_v+\frac{\rho_b}{\theta}C_v^*+C_cC_{vc}+\frac{\rho_b}{\theta}C_c^*C_{vc}^*\right)=D_{xv}\frac{\partial^2 C_v}{\partial x^2}+D_{xvc}\frac{\partial^2}{\partial x^2}(C_cC_{vc})+D_{yv}\frac{\partial^2 C_v}{\partial y^2}+D_{yvc}\frac{\partial^2}{\partial y^2}(C_cC_{vc})+D_{zv}\frac{\partial^2 C_v}{\partial z^2}+D_{zvc}\frac{\partial^2}{\partial z^2}(C_cC_{vc})-U\frac{\partial}{\partial x}(C_v+C_cC_{vc})-\lambda_vC_v-\lambda_{vc}C_vC_{vc}-\lambda_v^*\frac{\rho_b}{\theta}C_v^*-\lambda_{vc}^*\frac{\rho_b}{\theta}C_c^*C_{vc}^*+F_v$$

Reversible colloid adsorption 1st order equation
(Sim and Chrysikopoulos, 1998)

$$\frac{\rho_b}{\theta}\frac{\partial C_v^*(t,x,y,z)}{\partial t}=r_{v\text{-}v^*}C_v(t,x,y,z)-r_{v^*\text{-}v}\frac{\rho_b}{\theta}C_v^*(t,x,y,z)-\lambda_v^*\frac{\rho_b}{\theta}C_v^*(t,x,y,z)$$

The initial condition and the appropriate boundary conditions for the aquifer model employed in this study are as follows:

$$C_i(0,x,y,z)=0 \qquad \frac{\partial C_i^2(t,L_x,y,z)}{\partial x^2}=0$$

$$\frac{\partial C_i(t,x,0,z)}{\partial y}=\frac{\partial C_i(t,x,L_y,z)}{\partial y}=0$$

$$\frac{\partial C_i(t,x,y,0)}{\partial z}=\frac{\partial C_i(t,0,y,L_z)}{\partial z}=0$$

$$-D\frac{\partial C_i(t,0,y,z)}{\partial x}+UC_i(t,0,y,z)=\begin{cases}UC_{0i}, & t\le t_p\\ 0, & t>t_p\end{cases}$$

Model Simulations and fittings

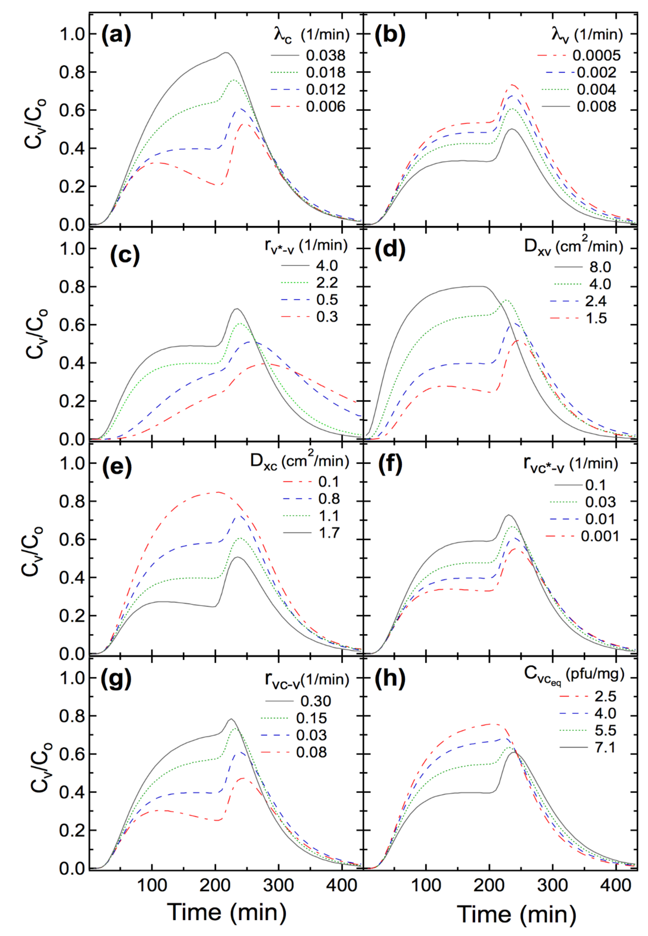

Figure 1

Figure 1: Sensitivity analysis of eight different parameters associated with the colloid facilitated virus transport model. The parameter values used are representative of the conditions employed in Exp. 1.

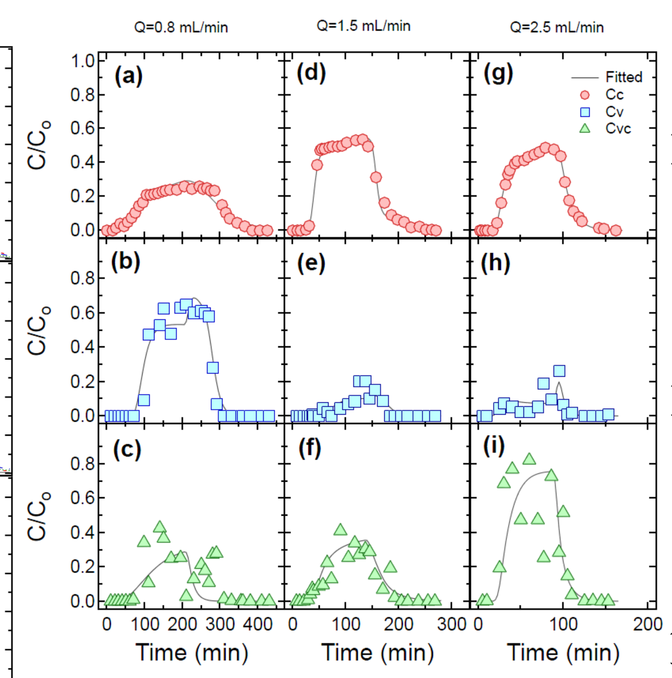

Figure 2

Figure 2: Experimental data from colloid facilitated virus transport (MS2-KGa1b) experiments in columns packed with glass beads. Figs 2a,b,c correspond to Exp. 1, Figs 2d,e,f to Exp. 2, and Figs 2g,h,i to Exp. 3. Colloid concentrations are represented by red circles, virus concentrations by blue squares, and virus-colloid complexes by green triangles. The solid black curves are the fitted model concentration histories.

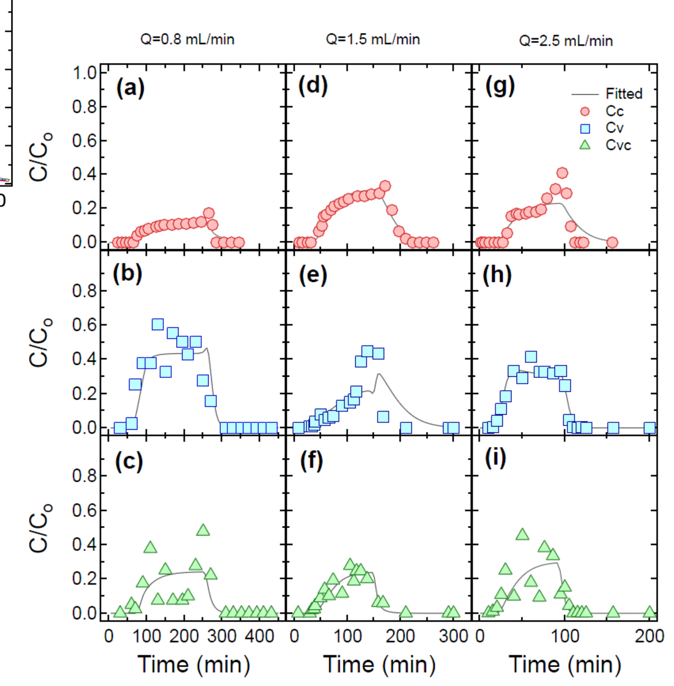

Figure 3

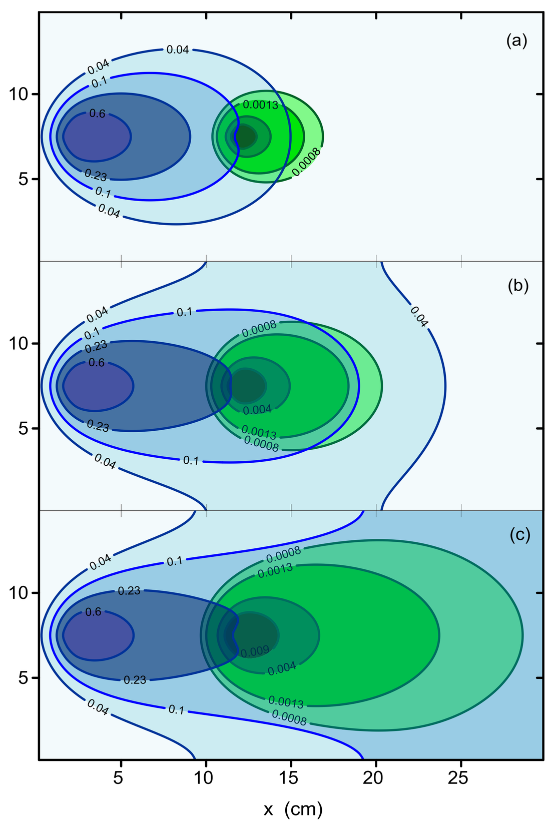

Figure 4

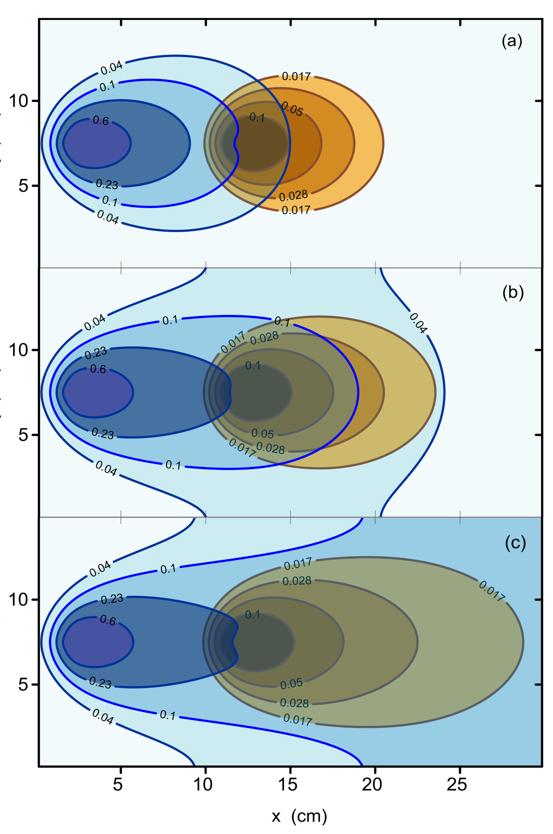

Figure 5

Figure 4: Contour plots on the x-y plane for model simulations of virus-colloid cotransport in a 3-D porous medium at (a) t=6 min, (b) 16 min, and (c) 30 min. Virus concentrations (pfu/mL) are indicated with blue colors and virus-colloid complex concentrations (pfu/mL) with green colors. The virus point source with constant concentration of 10 pfu/mL is located at (x,y,z)=(2.5, 7.45, 3,45 cm) whereas the colloid point source with constant concentration of 1.5 mg/mL is located at (x,y,z)=(12, 7.45, 3,45 cm). The dimensions of the porous medium are: Lx=30 cm, Ly=15 cm, and Lz=7.5 cm.

Figure 5: Contour plots on the x-y plane for model simulations of virus-colloid cotransport in a 3-D porous medium at (a) t=6 min, (b) 16 min, and (c) 30 min. Virus concentrations (pfu/mL) are indicated with blue colors and colloid concentrations (mg/mL) with brown colors. The virus point source with constant concentration of 10 pfu/mL is located at (x,y,z)=(2.5, 7.45, 3,45 cm) whereas the colloid point source with constant concentration of 1.5 mg/mL is located at (x,y,z)=(12, 7.45, 3,45 cm). The dimensions of the porous medium are: Lx=30 cm, Ly=15 cm, and Lz=7.5 cm.

Figure 3: Experimental data from ΦX174-KGa-1b experiment and model fits for colloid facilitated virus transport in glass beads porous media. Figs a,b,c refer to Exp. 4 model parameters, Figs d,e,f refer to Exp. 5 model data and Figs g,h,i refer to Exp. 6 model data. Three different normalized concentrations are presented: a) Colloid concentration (red circle), b) Virus concentration (blue square), c) Virus-colloid complex (purple triangle) concentration. Model fitted simulation (black line) used.

Notation

- F_i general form of species i source configuration, $[M_i/L^3t]$
- $r_{c\text{-}c^{*(r)}}$ attachment rate coefficient of colloids onto the solid matrix [1/t]
- $r_{c^{*(r)}\text{-}c}$ detachment rate coefficient of colloids from the solid matrix [1/t]
- $r_{c\text{-}c^{*(i)}}$ deposition rate coefficient of colloids onto the solid matrix [1/t]
- $r_{v\text{-}v^*}$ attachment rate coefficient of viruses onto the solid matrix [1/t]
- $r_{v^*\text{-}v}$ detachment rate coefficient of viruses from the solid matrix [1/t]
- λ_i decay rate of species i suspended in the liquid phase [1/t]
- λ_i^* decay rate of species i attached onto the solid matrix [1/t]
- D_{ij} hydrodynamic dispersion coefficient of species i, at the j direction $[L^2/t]$
- L_i Length of the i dimension of the aquifer medium [L]
- $r_{vc-v^*c^*}$ coefficient for attachment of suspended viruses-colloid particles onto the solid matrix [1/t]
- $r_{v^*c^*-vc}$ detachment rate coefficient for attached onto the solid matrix virus-colloid particles [1/t]
- $r_{v-v^*c^*}$ attachment rate coefficient of suspended viruses onto colloids (already attached onto solid matrix) $[M_c/M_vt]$
- $C_{vc_{eq}}$ concentration of viruses attached onto colloids already attached onto the solid matrix at equilibrium $[M_v/M_c]$
- $C^*_{vc_{eq}}$ concentration of viruses attached onto suspended colloid particles at equilibrium $[M_v/M_c]$
- r_{v-vc} attachment rate coefficient of suspended viruses onto suspended colloids particles $[M_c/M_v t]$
- $r_{v^*c^*-v}$ rate coefficient of virus detachment from virus-colloid particles attached onto the solid matrix [1/t]
- r_{vc-v} rate coefficient for virus detachment from suspended colloids [1/t]

The Fitting Process

For the estimation of the unknown parameters, the commercial code Pest was used to fit the experimental data with the one-dimensional transport model. Pest is Model-Independent Parameter Estimation software and can adjust model parameters or excitation data so that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum. For the needs of the fitting process some parameters were given from experiments in literature (status="Literature") while others had their values set, based on experimental data (status="Imposed") or physical laws (status="Fixed").

Application and results

The experimental data from colloid-facilitated virus transport experiments in packed columns, conducted by Syngouna and Chrysikopoulos (2013), were fitted by the newly developed model. MS2 (exp. 1-3) and ΦX174 (exp. 4-6) were used as model viruses, and kaolinite (kGa-1b) as model clay colloids. Interstitial velocity was set to 0.38 (exp. 1 and 4), 0.74 (exp. 2 and 5), and 1.21 (exp. 3 and 6) cm/min. Finally all cotransport experiments were conducted using a 30 cm long glass column with 2.5 cm diameter, which was packed with 2 mm diameter glass beads and placed horizontally.

Table 1 MS2-KGa1b (Exp. 1-3) and ΦX174-KGa-1b (Exp. 4-6) Fitted parameters

Parameter	Status	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 5	Exp. 6	Units
D_{xc}	Fitted	2.1±1.5	0.2±1.1	0.18±0.8	1.8E-3±1.1	0.038±0.2	0.036 ±0.8	cm^2/min
D_{xv}	Fitted	0.1±0.3	0.1±0.1	0.17±0.2	0.1±0.2	0.53±0.2	0.5±0.3	cm^2/min
D_{xvc}	Fitted	0.1±0.1	0.26±0.5	0.6±0.1	0.1±0.1	0.63±0.2	0.1±0.4	cm^2/min
U	Fixed	0.380	0.740	1.210	0.380	0.740	1.210	cm/min
θ	fixed	0.42	0.42	0.42	0.42	0.42	0.42	1/min
$r_{c\text{-}c^{*(i)}}$	Fixed	0.014±0.1	0.014±0.01	0.03±0.02	0.7E-02±0.2	0.028±0.002	0.058±0.02	1/min
$r_{c\text{-}c^{*(r)}}$	Literature	0.07	0.006	0.045	0.01	0.078	0.081	1/min
$r_{c^{*(r)}\text{-}c}$	Fitted	0.12±0.1	0.021±6.2	0.138±1.2	4.2E-2±0.2	0.112±0.1	0.12±1.1	1/min
ρ	Fixed	1610	1610	1610	1610	1610	1610	mg/cm^3

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