Cotransport of dense colloids and viruses in three-dimensional porous media

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Abstract

A three-dimensional numerical model was developed to investigate the simultaneous transport (cotransport) of dense colloids and viruses in homogeneous, water saturated, porous media with horizontal uniform flow. The dense colloids are assumed to exist in two different phases: suspended in the aqueous phase, and attached reversibly and/or irreversibly onto the solid matrix. The viruses are assumed to exist in four different phases: suspended in aqueous phase, attached onto the solid matrix, attached onto suspended colloids, and attached onto colloids already attached onto the solid matrix. The viruses in each of the four phases are assumed to undergo inactivation with different rates. Moreover, the suspended dense colloids as well as viruses attached onto suspended dense colloids are assumed to exhibit a "restricted" settling velocity as a consequence of the gravitational force; whereas, viruses due to their small sizes and densities are assumed to have negligible "restricted" settling velocity. The governing differential equations were solved numerically with the finite difference schemes, implicitly or explicitly implemented. Model simulations have shown that the presence of dense colloid particles can either enhance or hinder the horizontal transport of viruses, but also can increase the vertical migration of viruses

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.

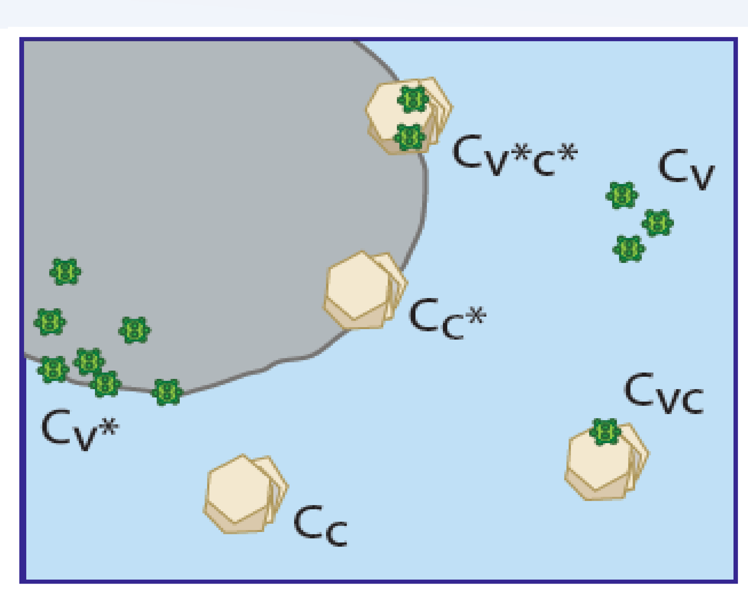

Figure 1: Schematic illustration of the six different concentrations accounted for, in the cotransport numerical model.

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) $[M_v/M_c]$

$C_{v^*c^*}$ Viruses attached onto colloid particles that are already attached onto the solid matrix (or virus-colloid particles attached onto the solid matrix) $[M_v/M_c]$

Mathematical model

Governing partial differential equations

3-D Colloid transport equation

(Katzourakis and Chrysikopoulos, 2014; Fabrice Compere et al., 2001)

$$\frac{\partial C_c(t,x,y,z)}{\partial t}+\frac{\rho_b}{\theta}\frac{\partial C_{c^*}(t,x,y,z)}{\partial t}-D_{xc}\frac{\partial^2 C_c(t,x,y,z)}{\partial x^2}-D_{yc}\frac{\partial^2 C_c(t,x,y,z)}{\partial y^2}-D_{zc}\frac{\partial^2 C_c(t,x,y,z)}{\partial z^2}$$
$$+\left(U_x+U_{cs(\pm i)}\right)\frac{\partial C_c(t,x,y,z)}{\partial x}+U_{cs(-k)}\frac{\partial C_c(t,x,y,z)}{\partial z}=F_c(t,x,y,z)$$

Colloid facilitated virus transport equation

(Vasiliadou and Chrysikopoulos, 2011; Katzourakis and Chrysikopoulos, 2014)

$$\frac{\partial}{\partial t}\left(C_v+\frac{\rho_b}{\theta}C_{v^*}+C_cC_{vc}+\frac{\rho_b}{\theta}C_{c^*}C_{v^*c^*}\right)=D_{xv}\frac{\partial^2 C_v}{\partial x^2}+D_{xvc}\frac{\partial^2}{\partial x^2}(C_cC_{vc})$$
$$+D_{yv}\frac{\partial^2 C_v}{\partial y^2}+D_{yvc}\frac{\partial^2}{\partial y^2}(C_cC_{vc})+D_{zv}\frac{\partial^2 C_v}{\partial z^2}+D_{zvc}\frac{\partial^2}{\partial z^2}(C_cC_{vc})$$
$$-\left(U_x+U_{vs(\pm \mathbf{i})}\right)\frac{\partial}{\partial x}(C_v+C_cC_{vc})-U_{vs(-\mathbf{k})}\frac{\partial}{\partial z}(C_v)-U_{vcs(-\mathbf{k})}\frac{\partial}{\partial z}(C_cC_{vc})$$
$$-\lambda_vC_v-\lambda_{vc}C_vC_{vc}-\lambda_{v^*}\frac{\rho_b}{\theta}C_{v^*}-\lambda_{v^*c^*}\frac{\rho_b}{\theta}C_{c^*}C_{v^*c^*}+F_v(t,x,y,z)$$

Suspended colloid-virus complex mass accumulation rate

(Bekhit et al., 2009)

$$\frac{\partial}{\partial t}(C_cC_{vc})=r_{v-vc}(C_c)^2C_v-r_{vc-v}(C_cC_{vc})+\frac{\rho_b}{\theta}r_{v^*c^*-vc}(C_{c^*}C_{v^*c^*})$$
$$-r_{vc-v^*c^*}(C_cC_{vc})-\lambda_{vc}C_cC_{vc}$$

Adsorbed colloid-virus complex mass accumulation rate

(Bekhit et al., 2009; Katzourakis and Chrysikopoulos, 2014)

$$\frac{\rho_b}{\theta}\frac{\partial}{\partial t}(C_{c^*}C_{v^*c^*})=\frac{\rho_b}{\theta}r_{v-v^*c^*}(C_{c^*})^2C_v-\frac{\rho_b}{\theta}r_{v^*c^*-v}(C_{c^*}C_{v^*c^*})+r_{vc-v^*c^*}(C_cC_{vc})$$
$$-\frac{\rho_b}{\theta}r_{v^*c^*-vc}(C_{c^*}C_{v^*c^*})-\lambda_{v^*c^*}\frac{\rho_b}{\theta}C_{c^*}C_{v^*c^*}$$

Reversible colloid adsorption 1st order equation

(Sim and Chrysikopoulos, 1998)

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

Irreversible colloid adsorption 1st order equation

(Compere et al., 2001)

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

Reversible virus adsorption 1st order equation

(Sim and Chrysikopoulos, 1998)

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

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

$$C_i(0,x,y,z)=0$$

$$-D\frac{\partial C_i(t,0,y,z)}{\partial x}+UC_i(t,0,y,z)=\begin{cases}UC_{0i}, & t\le t_p\\ 0, & t>t_p\end{cases}\qquad \frac{\partial C_i^2(t,L_x,y,z)}{\partial x^2}=0$$

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

The solution procedure

The classical Crank-Nikolson finite differences scheme was implemented, because its semi-implicit nature allows for both stability and accuracy. The resulting large system of algebraic equations was solved with the Pardiso package, which is a memory-efficient software, capable of solving sparse asymmetric and symmetric linear systems of equations (Schenk and Gärtner, 2004). The arising stiffness in the coupled systems were was with the sophisticated subroutine dodesol (Intel® Ordinary Differential Equations Solver Library), which is capable of solving ordinary differential equations (ODEs) with a variable or a priori unknown stiffness.

Model simulations

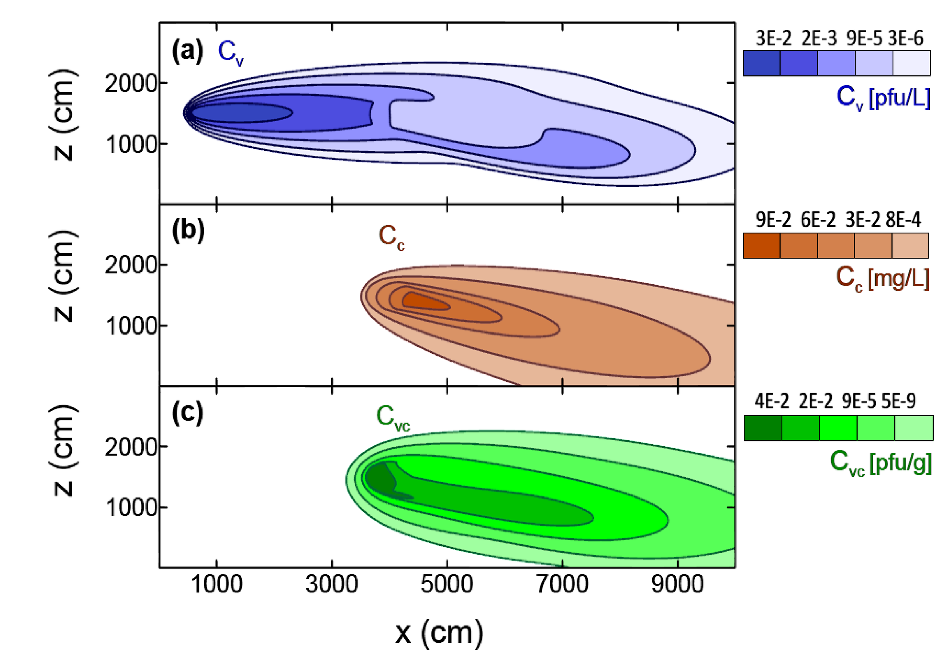

Figure 2. Concentration contour plots on the x-z plane for: (a) viruses, (b) colloids, and (c) virus-colloid particles during virus and colloid cotransport, accounting for gravitational effects. Here t=6900 hr, and y=15 m.

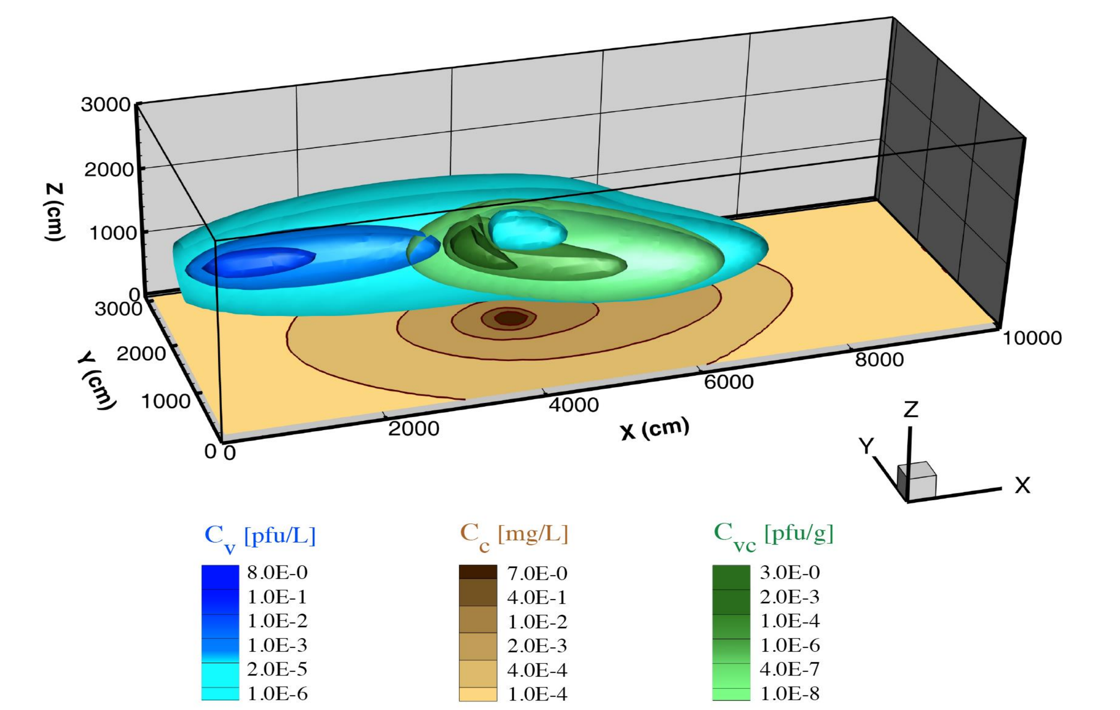

Figure 3. Concentration contour plots on the x-z plane for: (a) viruses, (b) colloids, and (c) virus-colloid particles during virus and colloid cotransport, accounting for gravitational effects. Here t=6900 hr, and y=15 m.

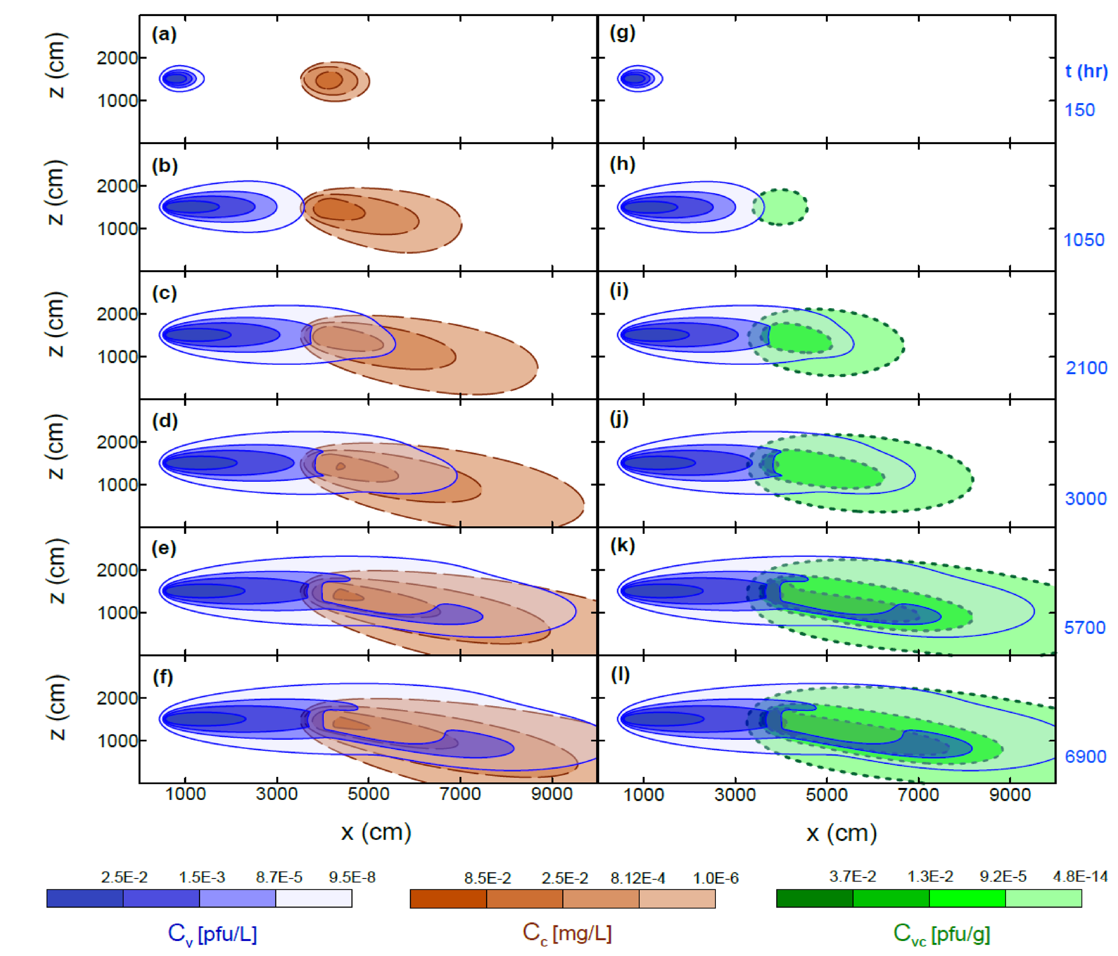

Figure 4. Contour plots on the x-z plane for: (a-f) viruses (solid curves) and colloid particles (dashed curves), and (g-l) viruses (solid curves) and virus-colloid particles (dotted curves) during virus and colloid cotransport in the presence of gravitational effects. Here (a,g) t=150 hr, (b,h) t=1050 hr, (c,i) t=2010 hr, (d,j) t=3000 hr, (e,k) t=5700 hr, (f,l) t=6900 hr, and y=15 m.

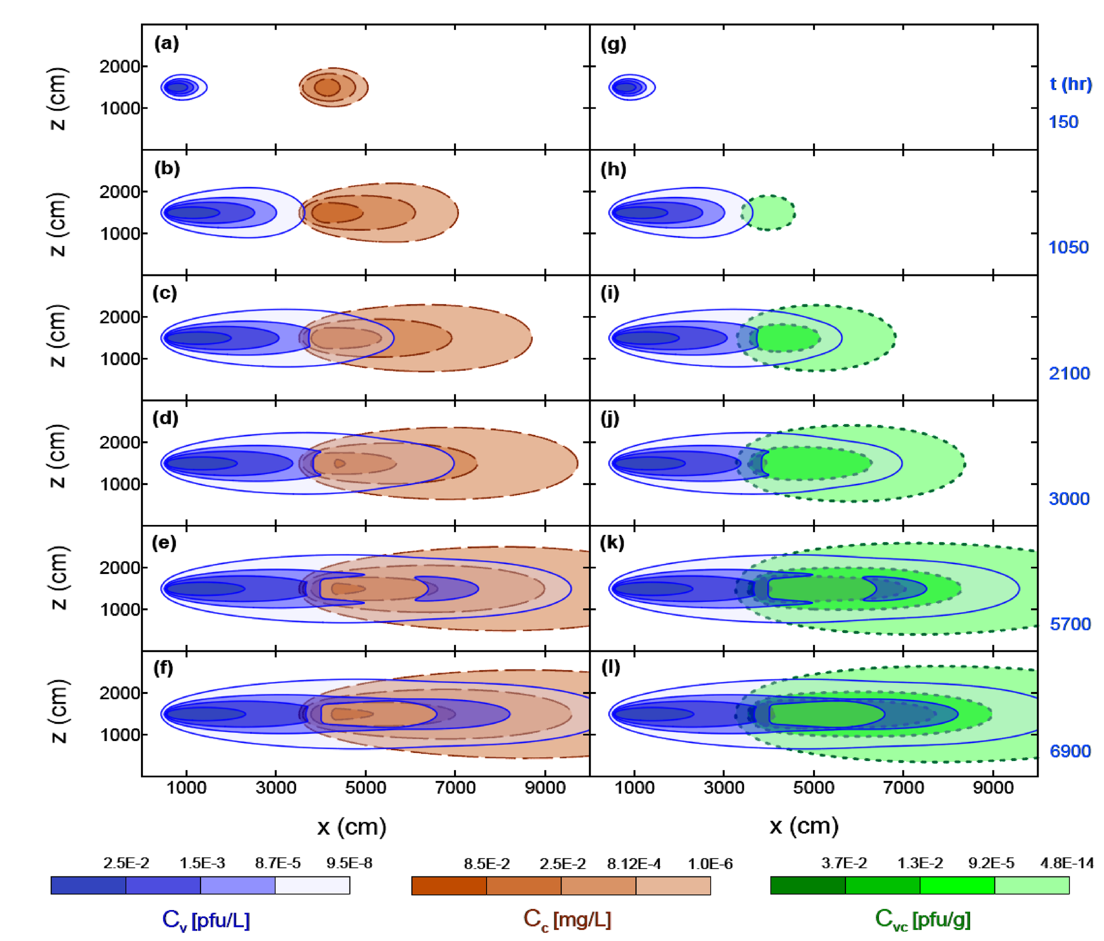

Figure 5. Contour plots on the x-z plane for: (a-f) viruses (solid curves) and colloid particles (dashed curves), and (g-l) viruses (solid curves) and virus-colloid particles (dotted curves) during virus and colloid cotransport in the absence of gravitational effects. Here (a,g) t=150 hr, (b,h) t=1050 hr, (c,i) t=2010 hr, (d,j) t=3000 hr, (e,k) t=5700 hr, (f,l) t=6900 hr, and y=15 m.

Summary

- A mathematical model describing the cotransport of viruses and colloids accounting for gravity effects was developed.
- An efficient numerical solution was implemented using implicit and non-implicit finite difference procedures, as well as ODE solvers.
- Multiple model simulations were performed particles in a hypothetical aquifer, using realistic parameter values reported in the literature.
- The results demonstrated that gravity, in the presence of dense colloids, greatly influences the transport of viruses in porous media.

Notation

F_i	general form of species i source configuration, $[M_i/L^3t]$	D_{ij}	hydrodynamic dispersion coefficient of species i, at the j direction $[L^2/t]$	λ_i	decay rate of species i suspended in the liquid phase [1/t]
L_i	Length of the i dimension of the aquifer medium [L]	r_{i-i^*}	attachment rate of species i onto the solid matrix [1/t]	λ_i^*	decay rate of species i attached onto the solid matrix [1/t]

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