Virus transport in saturated one-dimensional porous media

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ABSTRACT

A new mathematical model for virus transport in one-dimensional homogeneous, saturated porous media for a constant flux boundary condition is developed, accounting for first-order inactivation of suspended and filtered viruses with different inactivation constants. The virus attachment onto the solid matrix is considered as a filtration process which is suitable for viruses behaving as colloids. The closed-form analytical solutions are developed for a semi-infinite porous medium by Laplace transform techniques. The impact of the model parameters on virus transport is examined.

INTRODUCTION

Viruses are intracellular parasites that can be classified as colloid particles with size ranging from 0.02 μm to 0.3 μm [15]. They are generally negatively charged and vary widely in shape and chemical composition. A virus particle contains a nucleic acid, either DNA or RNA, which is surrounded by a protein coat (capsid) consisting of a number of protein molecules. These molecules are called capsomers and they are arranged in a precise and highly repetitive pattern around nucleic acid. Because viruses do not have their own respiratory and biosynthetic functions, they reproduce inside other cells by a process called infection. Viruses are classified on the basis of the hosts they infect. The three major groups of viruses are: animal viruses, plant viruses, and bacterial viruses (bacteriophages) [1]. The most common types of viruses found in groundwater are adenovirus, coliphage, coxsackievirus, enterovirus, hepatitis, poliovirus, and rotavirus, [6, 23]. These viruses can cause diseases such as gastroenteritis, hepatitis A, among others [4].

The transport and fate of viruses in porous media are mainly governed by virus attachment onto the solid matrix and inactivation [20]. Although a virus may undergo sorption via physical adsorption, chemical adsorption or ion
exchange, the major mechanism of virus attachment results from electrostatic double-layer interactions and van der Waals forces [16]. The virus attachment process is controlled by many factors, including temperature, microbial activity, moisture content, pH, and soil properties, to mention a few [23].

The colloid filtration theory is frequently applied to virus transport in porous media. Colloid filtration is a two stage process [9, 17, 22]. First, the solid matrix is coated by colloids through interception due to size differences between colloids and the solid matrix, sedimentation due to density differences between the fluid and colloids, and diffusion due to particles’ Brownian movement and surface forces. Subsequently, colloids may form aggregates which may break by the hydrodynamic drag force and redeposit onto other parts of the collector [17]. Generally, the interception and sedimentation processes (mechanical filtration) are effective only for large size particles (≥ 1 μm), so virus deposition is governed mainly by Brownian diffusion and the surface forces such as electrostatic and van der Waals forces (physicochemical filtration) [9]. Therefore, for the case of virus filtration, the effects of sedimentation and interception can be neglected [8].

Virus inactivation is defined as a loss of viral titer with time due to disruption of coat proteins, and degradation of nucleic acid [5]. Inactivation of suspended as well as sorbed or attached viruses is an irreversible sink mechanism that is commonly described by a first–order rate expression [23]. It has been reported that the inactivation rate is smaller for attached than suspended viruses [5, 10, 20, 23]. Thus, inactivation rates of suspended and attached viruses should not be assumed equal. The most important factor for virus inactivation in the subsurface is temperature [24]. Viruses remain infective much longer at lower temperatures (1 – 8°C) than at higher temperatures (20 – 32°C) [12]. Therefore, near the top layer of an unsaturated subsurface formation where temperature fluctuations occur, the inactivation rate must be considered as a variable rather than a constant parameter. Correlations of virus inactivation rates with temperature have been reported by Reddy et al. [13].

There are several mathematical models available in the literature for virus transport in porous media. Some of these models treat viruses as solutes due to their small size. Grosser [7] employed a one–dimensional advection/dispersion equation to describe virus transport in homogeneous porous media under local equilibrium conditions assuming equal inactivation rates for both adsorbed and suspended viruses. Tim and Mostaghimi [18] developed a numerical model for water flow and virus transport in variably saturated formations assuming that virus adsorption is an equilibrium process, and virus inactivation is identical for adsorbed as well as suspended viruses. Park et al. [12] developed a semi–analytical/numerical model (VIRALT) for both steady–state and transient vertical virus transport in the unsaturated zone and along the flowlines in the saturated zone, accounting for equilibrium adsorption and inactivation. Unlike the previous investigators, Vilker et al. [19] employed a nonequilibrium mass transfer process for viral adsorption to derive a model suitable for homogeneous packed column laboratory experiments under controlled steady–state flow conditions, by neglecting hydrodynamic dispersion and virus inactivation.

Several virus transport models have adopted the well established filtration theory to account for virus deposition onto the solid matrix. Corapcioglu and Haridas [3] derived a relatively complex filtration model for bacterial trans-

MATHEMATICAL MODEL

The one-dimensional virus transport in homogeneous, saturated porous media with first-order adsorption (or filtration) and inactivation is governed by the following partial differential equation

$$\frac{\partial C(t,x)}{\partial t} + \frac{\rho}{\theta} \frac{\partial C^*(t,x)}{\partial t} = D \frac{\partial^2 C(t,x)}{\partial x^2} - U \frac{\partial C(t,x)}{\partial x} - \lambda C(t,x) - \lambda^* \frac{\rho}{\theta} C^*(t,x),$$

(1)

where \(C\) is the concentration of virus in suspension; \(C^*\) is the mass of virus adsorbed on the solid matrix; \(D\) is the hydrodynamic dispersion coefficient; \(U\) is the average interstitial velocity; \(\rho\) is the bulk density of the solid matrix; \(\lambda\) is the inactivation constant of suspended viruses; \(\lambda^*\) is the inactivation constant of adsorbed viruses; \(\theta\) is the porosity of soil medium; \(t\) is time. The left hand side of the preceding equation consists of the accumulation terms, and the last two terms represent the inactivation of suspended and adsorbed viruses, respectively.

Assuming that the colloid filtration theory is applicable to virus transport, the rate of virus filtration is defined as [9]

$$\frac{\rho}{\theta} \frac{\partial C^*(t,x)}{\partial t} = k_c C(t,x) - k_r \frac{\rho}{\theta} C^*,$$

(2)

where \(C^*\) is now the virus concentration retained in the porous medium by the filtration process, and \(k_c\) is the clogging rate constant; \(k_r\) is the declogging rate constant. The rate of virus filtration depends on the interstitial velocity, suspended virus concentration and filter coefficient. Although colloid filtration is a time dependent process where deposited colloids may alter the surface structure as well as the porosity of the filtering medium and consequently lead to a variable filter coefficient, for the filtration of submicron particles like virus it is assumed that no change in the filter coefficient occur progressively in time. The clogging rate constant can be written as

$$k_c = U \phi F(C^*),$$

(3)

where \(\phi\) is the filter coefficient; and \(F(C^*)\) accounts for variations of porosity with increasing particle attachment. When there is no particle–particle interaction (“clean” media) \(F(C^*)\) is assumed to be one. The rate of declogging is
proportional to suspended particle concentration [14]; therefore, in the case of low suspended virus concentration declogging is negligible and (2) reduces to the well-known expression for irreversible colloid filtration

$$\frac{\rho}{\theta} \frac{\partial C^*(t, x)}{\partial t} = UC(t, x)\phi F(C^*). \quad (4)$$

For this special case the liquid-phase virus concentration is totally indifferent to the inactivation rate of irreversibly attached viruses.

The filter coefficient is an experimentally determined parameter, which for spherical filter particles of identical size is given by [17]

$$\phi = \frac{3(1 - \theta)\alpha \eta}{2d}, \quad (5)$$

where $d$ is the diameter of the filter material; $\alpha$ is the collision efficiency defined as the ratio of the number of the contacts producing adhesion to the number of collisions of the suspended particle with the filter material; and $\eta$ is the single collector efficiency, defined as the ratio of the rate at which particles strike the collector to the rate at which particles flow toward the collector. For a system where all suspended particles are completely destabilized, $\alpha = 1$ [15, 17]. The collector efficiency is expressed as [22]

$$\eta = \eta_d + \eta_g + \eta_i, \quad (6)$$

where $\eta_d$, $\eta_g$, and $\eta_i$ are the single collector efficiencies for Brownian diffusion, sedimentation, and interception filtration mechanism, respectively. For small particles like viruses the sedimentation and interception mechanisms can be neglected [21], and the single collector efficiency can be estimated by [22]

$$\eta = \eta_d = 0.9 \left( \frac{\sigma_B K}{\mu d_p \nu} \right)^{2/3}, \quad (7)$$

where $\eta_d$ is defined experimentally assuming that the suspended particles are spherical of identical sizes; $\sigma_B$ is the Boltzmann constant; $\mu$ is the viscosity of the fluid; $d_p$ is the diameter of the suspended particle; and $K$ is the absolute temperature.

The desired expression for $C^*$ is obtained by solving (2) subject to an initial condition of zero sorbed (or filtered) virus concentration ($C^*(0, x) = 0$) as

$$C^*(t, x) = \frac{r_1 \theta}{\rho} \int_0^t C(\tau, x) \exp \left[ -\frac{r_2 \theta}{\rho} (t - \tau) \right] d\tau, \quad (8)$$

where the following substitutions have been employed

$$r_1 = k_e, \quad r_2 = \frac{k_e \rho}{\theta}. \quad (9a, b)$$

In the view of (2), (8) and (9) the governing equation (1) can be written as

$$\frac{\partial C(t, x)}{\partial t} = D \frac{\partial^2 C(t, x)}{\partial x^2} - UC(t, x) \frac{\partial C(t, x)}{\partial x} - AC(t, x) - B \int_0^t C(\tau, x) e^{-\mathcal{K}(t-\tau)} d\tau, \quad (10)$$
where the following substitutions have been employed

\[ A = r_1 + \lambda, \quad B = r_1(\lambda^* - \mathcal{H}), \quad \mathcal{H} = \frac{\theta r_2}{\rho}. \]  

(11a, b, c)

For a semi–infinite one–dimensional porous medium in the presence of a continuous source of viruses, the appropriate initial and boundary conditions are

\[ C(0, x) = 0, \]

(12)

\[ -D \frac{\partial C(t, 0)}{\partial x} + UC(t, 0) = UC_0, \]

(13)

\[ \frac{\partial C(t, \infty)}{\partial x} = 0, \]

(14)

where \( C_0 \) is the source concentration. The condition (12) establishes that there is no initial virus concentration within the one–dimensional porous medium. The constant flux boundary condition (13) implies virus concentration discontinuity at the inlet. The downstream boundary condition (14) preserves concentration continuity for a semi–infinite system. Equation (10) subject to conditions (12)-(14) is solved analytically following the methods of Chrysikopoulos et al. [2].

Taking Laplace transforms with respect to time variable \( t \) and space variable \( x \), using the transformed boundary conditions and applying inverse transformations yields

\[ C(t, x) = \frac{C_0 U}{D^{1/2}} \exp \left[ \frac{Ux}{2D} \right] \times \]

\[ \left\{ \int_0^t \int_0^\infty \mathcal{H} e^{-\mathcal{H} \tau} J_0 \left[ 2\sqrt{B \zeta(t - \zeta)} \right] \left[ \frac{1}{(\pi \zeta)^{1/2}} \exp \left[ -\frac{x^2}{4D\zeta} + \left( \mathcal{H} - A - \frac{U^2}{4D} \right) \zeta \right] \right] d\zeta d\tau \right. \]

\[ - \frac{U}{2D^{1/2}} \exp \left[ \frac{Ux}{2D} + (\mathcal{H} - A)\zeta \right] \text{erfc} \left[ \frac{x}{2(D\zeta)^{1/2}} + \frac{U}{2} \left( \frac{\zeta}{D} \right)^{1/2} \right] \right\} \]

\[ + e^{-\mathcal{H}t} \int_0^t J_0 \left[ 2\sqrt{B \zeta(t - \zeta)} \right] \left[ \frac{1}{(\pi \zeta)^{1/2}} \exp \left[ -\frac{x^2}{4D\zeta} + \left( \mathcal{H} - A - \frac{U^2}{4D} \right) \zeta \right] \right] d\zeta \]

\[ - \frac{U}{2D^{1/2}} \exp \left[ \frac{Ux}{2D} + (\mathcal{H} - A)\zeta \right] \text{erfc} \left[ \frac{x}{2(D\zeta)^{1/2}} + \frac{U}{2} \left( \frac{\zeta}{D} \right)^{1/2} \right] \right\}, \]

(15)

where \( J_0 \) is the Bessel function of the first kind of zeroth order.

Model Simulations

To illustrate the effect of the parameters of the newly developed transport model, temporal and spatial virus distributions have been calculated for a variety of situations. For presentation purpose, calculated concentrations were normalized
by the source concentration. The integrals in (15) were evaluated by the extended Simpson’s rule. Unless otherwise specified, breakthrough curves are predicted at a distance $x = 9$ cm downstream from the source. The fixed parameter values used for the calculations are: $t=240$ hr, $D=15$ cm$^2$/hr, $U=4$ cm/hr, $\lambda=0.006$ d$^{-1}$, $\lambda^*=0.003$ d$^{-1}$, $\rho=1.5$ g/cm$^3$, and $\theta=0.25$.

The results from several model simulations indicate the intuitive result that the suspended virus concentration decreases with increasing inactivation constant of suspended viruses ($\lambda$), and that the suspended virus concentration decreases with increasing inactivation constant of adsorbed viruses ($\lambda^*$). Normalized concentration profiles for three different clogging and declogging rate constants have been presented in Figure 1 and Figure 2, respectively. These snapshots indicate
that the suspended virus concentration increases with decreasing clogging rate constant \((k_c)\) and increasing declogging rate constant \((k_r)\), due to the decreased amount of filtered viruses.

**SUMMARY**

An analytical model for One-dimensional virus transport homogeneous porous media is presented, and some of the features of the model are illustrated. The model accounts for first-order rate inactivation of suspended and attached viruses and virus attachment by a filtration process. The governing partial differential equations were solved analytically for a constant flux boundary conditions using Laplace transform techniques. The effect of model parameters on liquid-phase virus concentration was investigated. The virus concentration was found to be mostly sensitive to the clogging/declogging rate constants as well as to the inactivation rate constants. Although the model presented has many advantages due to its analytical nature, some of the limitations inherent to the model are its inability: (a) to allow for spatially variable velocity field; and (b) to account for the more realistic case of time dependent filtration.

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**REFERENCES**


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