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 Syngnou and Chrysikopoulos (2013) were satisfactorily fitted by the newly developed cotransport model.

Governing partial differential equations

3-D Colloid transport equation

\[ \frac{\partial (C_{v} C_{b})}{\partial t} + \frac{\partial (C_{v} u_{v} C_{b})}{\partial x} + \frac{\partial (C_{v} v_{v} C_{b})}{\partial y} + \frac{\partial (C_{v} w_{v} C_{b})}{\partial z} = D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial x^{2}} + D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial y^{2}} + D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial z^{2}} \]

Colloid facilitated virus transport equation

\[ \frac{\partial (C_{v} C_{b})}{\partial t} + \frac{\partial (C_{v} u_{v} C_{b})}{\partial x} + \frac{\partial (C_{v} v_{v} C_{b})}{\partial y} + \frac{\partial (C_{v} w_{v} C_{b})}{\partial z} = D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial x^{2}} + D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial y^{2}} + D_{v} \frac{\partial^{2} (C_{v} C_{b})}{\partial z^{2}} - k_{c} C_{v} C_{b} \]

Adsorbed colloid-virus complex mass accumulation rate

\[ \frac{d}{dt} (C_{v} C_{b}) = \frac{1}{\rho} \left[ (r_{v} - r_{c}) C_{v} C_{b} - (r_{v} - r_{c}) C_{v} C_{b} \right] \]

Irreversible colloid adsorption 1st order equation

\[ \frac{d}{dt} C_{v} = -k_{c} C_{v} \]

Reversible colloid adsorption 1st order equation

\[ \frac{d}{dt} C_{v} = -k_{c} C_{v} + k_{c} C_{v} \]

Reversible virus adsorption 1st order equation

\[ \frac{d}{dt} C_{v} = -k_{c} C_{v} \]

The Fitting procedure

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="Fixed").

Results

The experimental data from colloid-facilitated virus transport experiments in packed columns, conducted by Syngnou and Chrysikopoulos (2013), were fitted by the newly developed model. MS2 (exp. -1 and 3) and K97-1b (exp. -4 and 6) were used as model viruses, and kaolinite (KaS-1b) as model clay colloids. Supplimental fittings were also carried out on montmorillonite (STX-1b). Intertial 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.

References


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