Supporting Information

Effect of gravity on colloid transport through water-saturated columns packed with glass beads: Modeling and experiments

by

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Classification of modelling approaches

There are numerous mathematical models available that describe colloid transport in fractured and porous media. These models rely on either continuum or statistical approaches. Continuum approaches are based on macroscopically derived conservation equations and do not consider the morphology of the pore space within the solid matrix. Continuum approaches are divided into two groups: (a) phenomenological models, which make use of several parameters that may not be possible to estimate independently due to insufficient experimental data, and (b) trajectory based models, which use force balances to compute the actual paths of the colloids in the pore space. Statistical approaches account for the morphology of the pore space, and thus require relatively large computational power. The statistical approaches are divided into two groups: (a) random processes (Markov processes) or queueing theory (birth-death processes), and (b) network models. In this study, the frequently employed continuum approach was adopted, and the phenomenological colloid transport model developed by Sim and Chrysikopoulos[1] was extended to account for colloid sedimentation.

Definition sketch

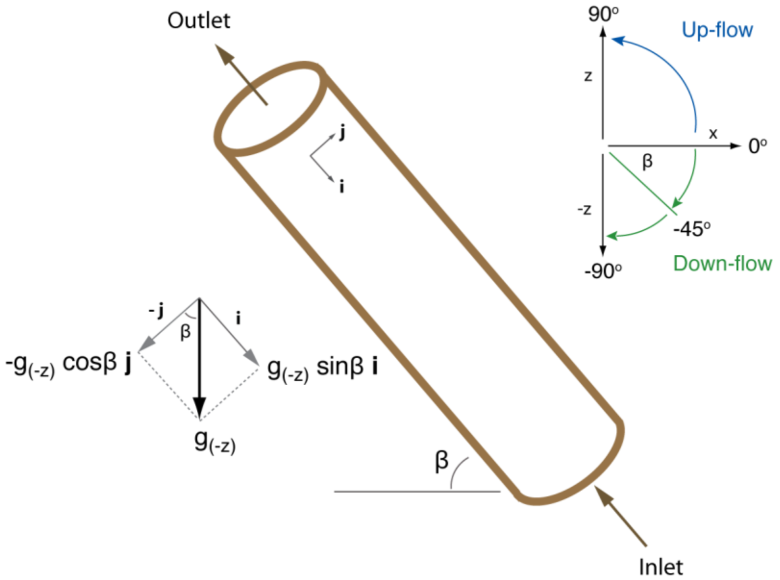

Figure SI1. Schematic illustration of a packed column with up-flow velocity having orientation (-**i**) with respect to gravity. The gravity vector components are: $g_{(i)} = g_{(-z)}$ sinβ **i,** and $g_{(-j)} = -g_{(-z)}$ cosβ **j.**

Analytical Solution

The analytical solution to the governing colloid transport equation (1) in conjunction with relationship (6), subject to conditions (7)-(9), with U instead of U_{tot}, has been derived by Sim and Chrysikopoulos:[1]

$$C(t,x) = \begin{cases} \Omega(t,x) & 0 < t \leq t_p \\ \Omega(t,x) - \Omega(t-t_p,x) & t > t_p \end{cases} \tag{SI1}$$

where

$$\begin{aligned}
\Omega(t,x) = \frac{C_0 U_{tot}}{D^{1/2}} \exp\left[\frac{U_{tot}x}{2D}\right] \Bigg\{ & \int_0^t \int_0^\tau H e^{-H\tau} J_0\left[2\left(B\xi(\tau-\xi)\right)^{1/2}\right] \\
& \cdot \left\{ \frac{1}{(\pi\xi)^{1/2}} \exp\left[\frac{-x^2}{4D\xi} + \left(H - A - \frac{U_{tot}^2}{4D}\right)\xi\right] \right. \\
& - \frac{U_{tot}}{2D^{1/2}} \exp\left[\frac{U_{tot}x}{2D} + (H-A)\xi\right] \\
& \left. \cdot \operatorname{erfc}\left[\frac{x}{2(D\xi)^{1/2}} + \frac{U_{tot}}{2}\left(\frac{\xi}{D}\right)^{1/2}\right] \right\} d\xi \, d\tau \\
& + e^{-Ht} \int_0^t J_0\left[2\left(B\xi(t-\xi)\right)^{1/2}\right] \\
& \cdot \left\{ \frac{1}{(\pi\xi)^{1/2}} \exp\left[\frac{-x^2}{4D\xi} + \left(H - A - \frac{U_{tot}^2}{4D}\right)\xi\right] \right. \\
& - \frac{U_{tot}}{2D^{1/2}} \exp\left[\frac{U_{tot}x}{2D} + (H-A)\xi\right] \\
& \left. \cdot \operatorname{erfc}\left[\frac{x}{2(D\xi)^{1/2}} + \frac{U_{tot}}{2}\left(\frac{\xi}{D}\right)^{1/2}\right] \right\} d\xi \Bigg\}.
\end{aligned} \tag{SI2}$$

where $A=k_c+\lambda$, $B=k_c k_r \theta/\rho$, $H=(k_c\theta/\rho)+\lambda^*$,[2] J_0 is the Bessel function of the first-kind of zeroth-order, and ξ and τ are dummy integration variables.

References

(1) Sim, Y.; Chrysikopoulos, C. V., Analytical models for one-dimensional virus transport in saturated porous media. *Water. Resour. Res*. **1995**, *31*, 1429–1437, DOI 10.1029/95WR00199. (Correction, *Water Resour. Res.*, **1996**, *32*, 1473, DOI 10.1029/96WR00675).

(2) Sim, Y.; Chrysikopoulos, C. V. Three-dimensional analytical models for virus transport in saturated porous media. *Transport in Porous Media* **1998**, *30*, 87–112, DOI 10.1023/A:1006596412177.