Research and Development

Building a scientific foundation for sound environmental decisions
One-Dimensional Variably Saturated Microbial Transport Simulations

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USGS/EPA STARS Grant Meeting on Cryptosporidium Removal by Bank filtration
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Collaborators

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Outline

Modeling goals

Conceptual model

Governing equations and their solution

Monte Carlo Simulations and sensitivity analyses

Conclusions/Questions
Modeling Goals

Motivated by
Ground Water Rule:
Physically based
Probabilistic
Modeling Goals

Predict probability of viable viruses passing through soil to reach water supply aquifer
Modeling Goals

Predict probability of viable viruses passing through soil to reach water supply aquifer
Conceptual model

- Air
- Liquid
- Solid
- Inactivation
- Mass transfer
- Soil layer
- $C_{irr}$
- $k_a$
- $k_s$
- $\lambda_a$
- $\lambda_s$
- $\lambda$
- $\theta$
- $z$
- $L$
- $\bar{v}C$
Governing equations

\[
\frac{\partial C}{\partial t} + \rho \frac{\partial C_s}{\partial t} + \frac{\partial C_a}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - \bar{v} \frac{\partial C}{\partial z} - C \lambda - \rho C_s \lambda_s - C_a \lambda_a
\]

\[
\rho \frac{\partial C_a}{\partial t} = k_s \theta \left( C - \frac{C_s}{K_d} \right) - \lambda_s \rho C_s
\]

\[
\theta \frac{\partial C_a}{\partial t} = k_a \theta C - \lambda_a \theta C_a
\]

Initial and boundary conditions

\[ C(0, z) = C_s(0, z) = C_a(0, z) = 0 \]

\[ \bar{v}c_o = -D \frac{\partial C}{\partial z} \bigg|_{z=0} + \bar{v}C \bigg|_{z=0} \]

\[ z \in [0, \infty) \]

\[ \frac{\partial C(t, z \to \infty)}{\partial z} = 0 \]
Method of solution

\[ A = \frac{M_r}{M_o} \]

\[ M_o = \int_0^\omega c_o(0, t)\bar{v}d\omega \quad \omega \to \infty \]

\[ M_r = \int_0^\omega f(z, t)d\omega \quad \omega \to \infty \]

\[ \lim_{t \to \infty} M_r = \lim_{s \to 0} s\tilde{M}(s, z) \]

\[ \tilde{M}_r = \frac{\tilde{f}(z, s)}{s} \]
Air-water interfacial area

Rose and Bruce (1949)*

\[ a_a = \frac{\rho_w g \theta h(\theta)}{\alpha \sigma} \]

Air-water interfacial area

![Graph showing Air-water interfacial area vs Se]

Kim et al. (1997) †

Anwar et al. (2000): ‡
- 25 mm, \( \log K_S = -0.165 \)
- 50 mm, \( \log K_S = -0.082 \)
- 75 mm, \( \log K_S = -0.029 \)


# Database of soil parameter distributions

## Table 1: Hydraulic Properties of Sand, Silt, and Clay

<table>
<thead>
<tr>
<th>Soil Type</th>
<th>Parameter</th>
<th>N</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>sand</td>
<td>( \theta_r )</td>
<td>308</td>
<td>0.050</td>
<td>0.003</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>sand</td>
<td>( \theta_s )</td>
<td>308</td>
<td>0.367</td>
<td>0.032</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>sand</td>
<td>( \log_{10} K_{s} )</td>
<td>99†</td>
<td>-0.691</td>
<td>0.218</td>
<td>( \log(m \text{ hr}^{-1}) )</td>
</tr>
<tr>
<td>sand</td>
<td>( \log_{10} \alpha )</td>
<td>308</td>
<td>0.5306</td>
<td>0.034</td>
<td>( \log(m^{-1}) )</td>
</tr>
<tr>
<td>sand</td>
<td>( \log_{10} \gamma )</td>
<td>308</td>
<td>0.482</td>
<td>0.077</td>
<td>( \log(\text{dimensionless}) )</td>
</tr>
<tr>
<td>sand</td>
<td>( \rho )</td>
<td>168§</td>
<td>1.58 \times 10^6</td>
<td>1.42 \times 10^5</td>
<td>( g \text{ m}^{-3} )</td>
</tr>
<tr>
<td>sand</td>
<td>( r_p )</td>
<td>0§</td>
<td>4.71 \times 10^{-4}</td>
<td>1.60 \times 10^{-5}</td>
<td>( m )</td>
</tr>
<tr>
<td>sand</td>
<td>( \sigma_s )</td>
<td>1†</td>
<td>5.59 \times 10^{-3}</td>
<td>0.00</td>
<td>( m )</td>
</tr>
<tr>
<td>sand</td>
<td>( T )</td>
<td>1944*</td>
<td>11.7</td>
<td>7.38</td>
<td>° Celsius</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \theta_r )</td>
<td>330</td>
<td>0.063</td>
<td>0.013</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \theta_s )</td>
<td>330</td>
<td>0.406</td>
<td>0.050</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \log_{10} K_{s} )</td>
<td>75†</td>
<td>-2.160</td>
<td>-0.384</td>
<td>( \log(m \text{ hr}^{-1}) )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \log_{10} \alpha )</td>
<td>330</td>
<td>-0.207</td>
<td>0.075</td>
<td>( \log(m^{-1}) )</td>
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<tr>
<td>silt loam</td>
<td>( \log_{10} \gamma )</td>
<td>330</td>
<td>0.206</td>
<td>0.016</td>
<td>( \log(\text{dimensionless}) )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \rho )</td>
<td>133§</td>
<td>1.43 \times 10^6</td>
<td>1.48 \times 10^5</td>
<td>( g \text{ m}^{-3} )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( r_p )</td>
<td>0§</td>
<td>1.18 \times 10^{-4}</td>
<td>5.50 \times 10^{-5}</td>
<td>( m )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( \sigma_s )</td>
<td>1†</td>
<td>8.75 \times 10^{-5}</td>
<td>0.00</td>
<td>( m )</td>
</tr>
<tr>
<td>silt loam</td>
<td>( T )</td>
<td>1944*</td>
<td>11.7</td>
<td>7.38</td>
<td>° Celsius</td>
</tr>
<tr>
<td>clay</td>
<td>( \theta_r )</td>
<td>84</td>
<td>0.101</td>
<td>0.011</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>clay</td>
<td>( \theta_s )</td>
<td>84</td>
<td>0.515</td>
<td>0.085</td>
<td>( L^2 L^{-3} )</td>
</tr>
<tr>
<td>clay</td>
<td>( \log_{10} K_{s} )</td>
<td>22†</td>
<td>-2.085</td>
<td>0.0475</td>
<td>( \log(m \text{ hr}^{-1}) )</td>
</tr>
<tr>
<td>clay</td>
<td>( \log_{10} \alpha )</td>
<td>84</td>
<td>0.276</td>
<td>0.129</td>
<td>( \log(m^{-1}) )</td>
</tr>
<tr>
<td>clay</td>
<td>( \log_{10} \gamma )</td>
<td>84</td>
<td>0.114</td>
<td>0.015</td>
<td>( \log(\text{dimensionless}) )</td>
</tr>
<tr>
<td>clay</td>
<td>( \rho )</td>
<td>38§</td>
<td>1.29 \times 10^6</td>
<td>1.68 \times 10^5</td>
<td>( g \text{ m}^{-3} )</td>
</tr>
<tr>
<td>clay</td>
<td>( r_p )</td>
<td>0§</td>
<td>9.95 \times 10^{-5}</td>
<td>6.15 \times 10^{-5}</td>
<td>( m )</td>
</tr>
<tr>
<td>clay</td>
<td>( \sigma_s )</td>
<td>1†</td>
<td>8.75 \times 10^{-5}</td>
<td>0.00</td>
<td>( m )</td>
</tr>
<tr>
<td>clay</td>
<td>( T )</td>
<td>1944*</td>
<td>11.7</td>
<td>7.38</td>
<td>° Celsius</td>
</tr>
</tbody>
</table>

* Generated with the Rosetta program (Schaap et al. 1999); unless otherwise noted.
† Field lysimeter study by Poleiška et al. (1995).
‡ Kaczmarek et al. (1997).
§ Data from Remote Soil Temperature Network [1].
¶ From the UNSODA database (Lei et al. 1996).
|| Generated with random deviates in soil textural triangle queried by USDA category.
# Database of virus parameter distributions

## Table 2: Parameters Used for Poliovirus

<table>
<thead>
<tr>
<th>Parameter*</th>
<th>N</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\log_{10} \lambda$</td>
<td>12</td>
<td>0.605</td>
<td>0.608</td>
<td>$\log(hr^{-1})$</td>
</tr>
<tr>
<td>$\log_{10} \lambda^*$</td>
<td>0‡</td>
<td>0.304</td>
<td>0.608</td>
<td>$\log(hr^{-1})$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>1†</td>
<td>$1.34 \times 10^{-3}$</td>
<td>$1.80 \times 10^{-3}$</td>
<td>$m \ hr^{-1}$</td>
</tr>
<tr>
<td>$\kappa^*$</td>
<td>1†</td>
<td>$9.27 \times 10^{-3}$</td>
<td>$1.80 \times 10^{-3}$</td>
<td>$m \ hr^{-1}$</td>
</tr>
<tr>
<td>$r_v$</td>
<td>0§</td>
<td>$1.375 \times 10^{-8}$</td>
<td>$1.25 \times 10^9$</td>
<td>$m^3 \ g^{-1}$</td>
</tr>
<tr>
<td>$K_d$ (sand)</td>
<td>87</td>
<td>$2.43 \times 10^{-4}$</td>
<td>$5.66 \times 10^{-4}$</td>
<td>$m^3 \ g^{-1}$</td>
</tr>
<tr>
<td>$K_d$ (silt loam)</td>
<td>23</td>
<td>$3.77 \times 10^{-4}$</td>
<td>$7.16 \times 10^{-4}$</td>
<td>$m^3 \ g^{-1}$</td>
</tr>
<tr>
<td>$K_d$ (clay)</td>
<td>39</td>
<td>$7.20 \times 10^{-4}$</td>
<td>$9.74 \times 10^{-4}$</td>
<td>$m^3 \ g^{-1}$</td>
</tr>
</tbody>
</table>

* Data complied by Breidenbach et al. (2001) unless otherwise noted.
† From Chu et al. (2001), see Appendix A for assumptions.
‡ Yates and Ouyang (1992) assumed $\lambda^* \approx \lambda/2$.
Virulo

http://www.epa.gov/ada/
Results of sensitivity analyses
Results of Monte Carlo Simulations

- **Clay**: $\mathbb{P}(A > \varepsilon) = 0.0067$
- **Clay Loam**: $\mathbb{P}(A > \varepsilon) = 0.0031$
- **Loam**: $\mathbb{P}(A > \varepsilon) = 0.0021$
- **Sandy Loam**: $\mathbb{P}(A > \varepsilon) = 0.0039$
- **Loamy Sand**: $\mathbb{P}(A > \varepsilon) = 0.0009$
- **Sand**: $\mathbb{P}(A > \varepsilon) = 0.0007$
Conclusions/Questions

- Laplace transform solution of advection-dispersion type equation
- Monte Carlo method
- Hydraulic conductivity and air-water interface most important

Publications: http://www.epa.gov/ada/

Predicting Attenuation of Viruses During Percolation in Soils:

1. Probabilistic Model (EPA/600/R-02/051a)
2. User’s Guide to the Virulo 1.0 Computer Model (EPA/600/R-02/051b)