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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Outline

Modeling goals

Conceptual model

Governing equations and their solution

Monte Carlo Simulations and sensitivity analyses

Conclusions/Questions

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Modeling Goals

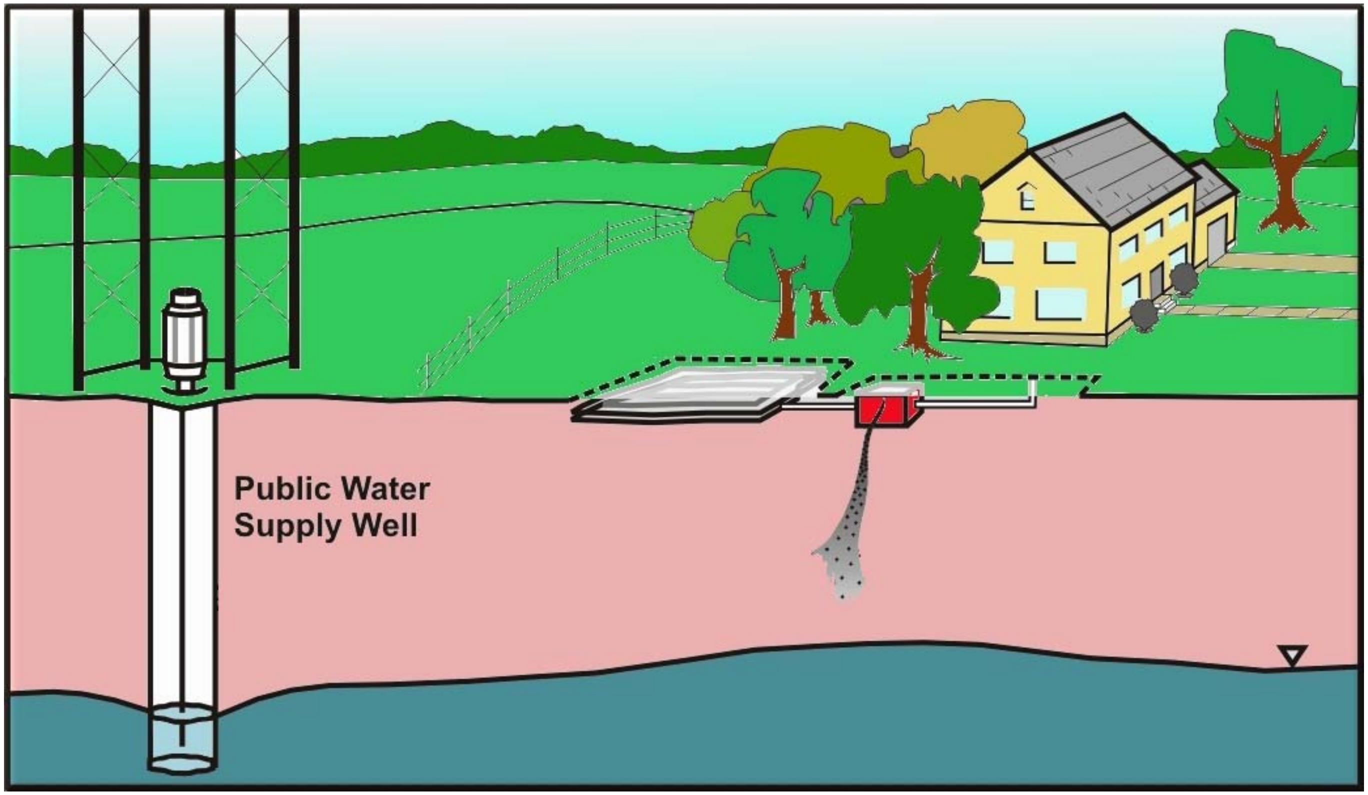
Motivated by
Ground Water Rule:

Physically based

Probabilistic

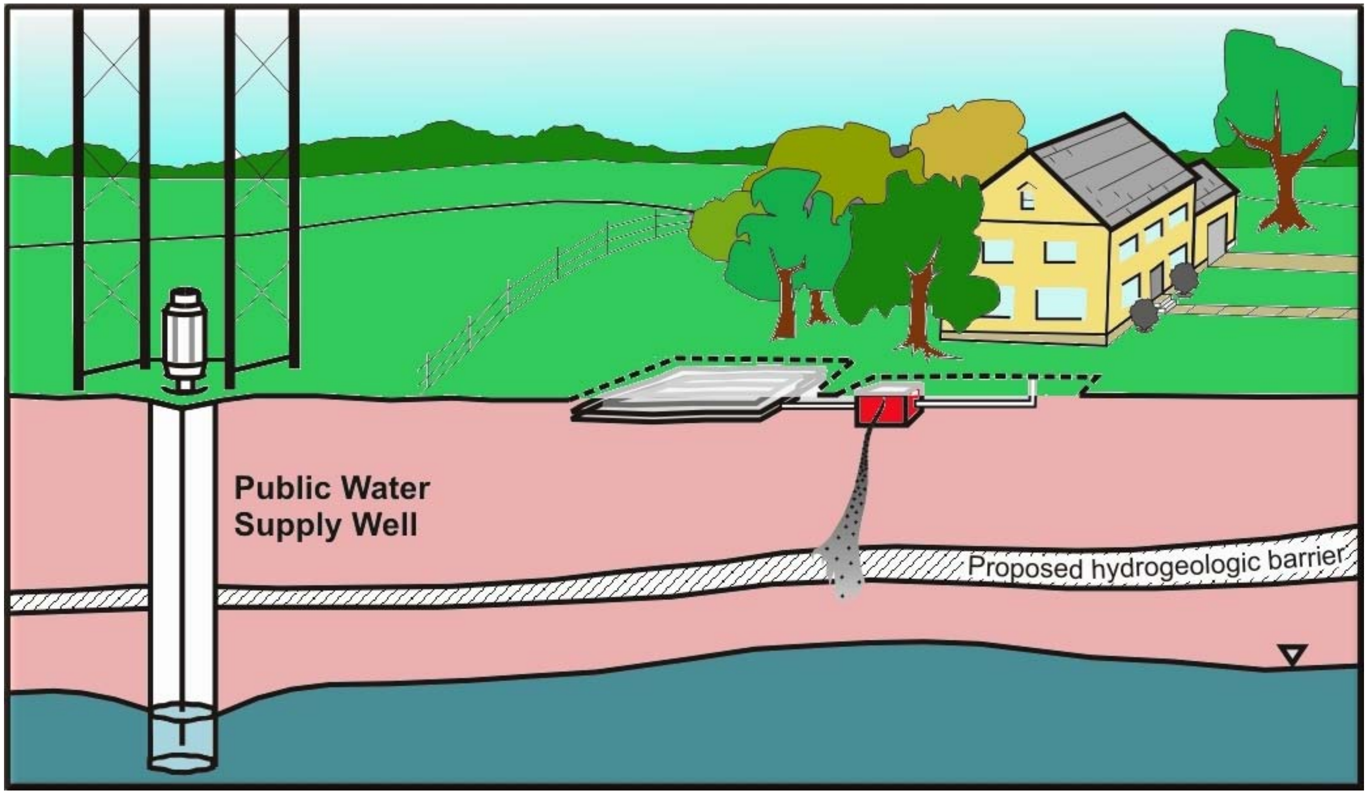
Modeling Goals

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



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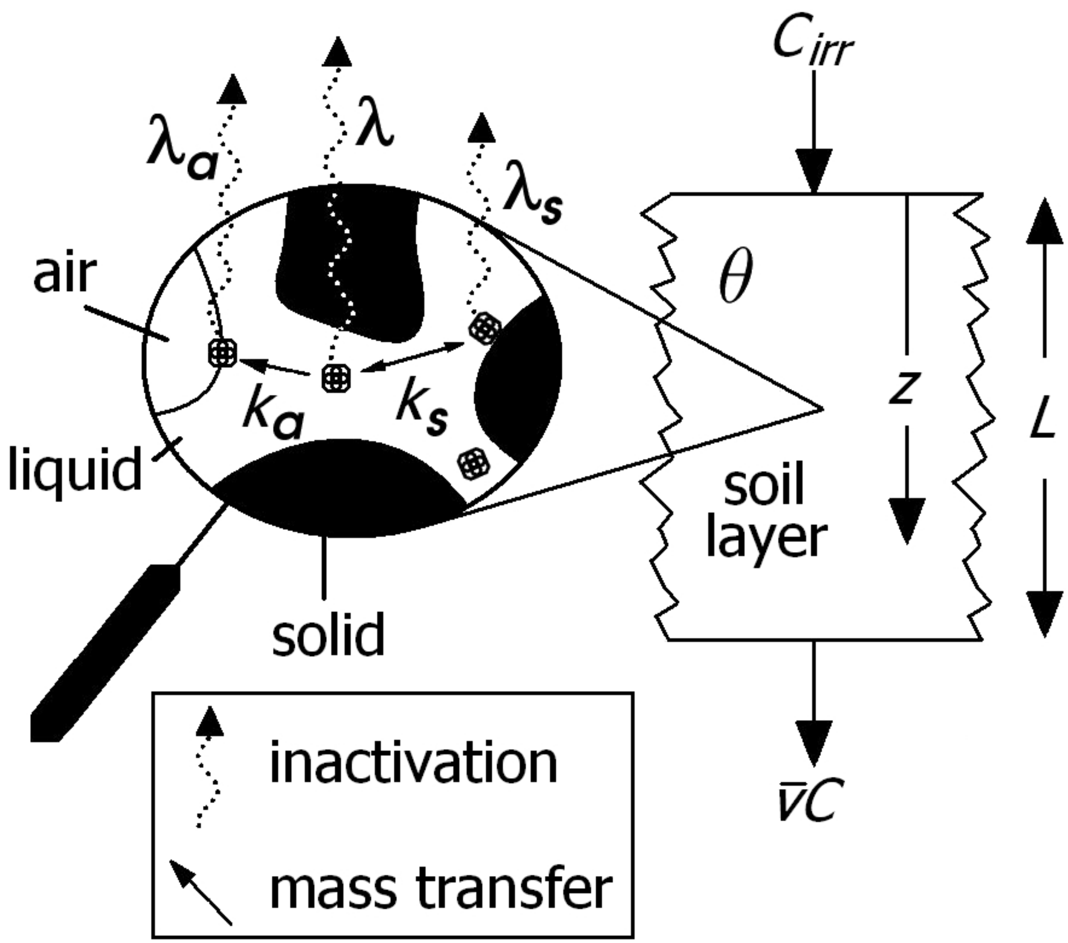
Conceptual model



Governing equations

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

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

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

Sim Y, Crysikopoulos CV, 2000. Virus transport in unsaturated porous media. Water Resources Research 36(1):173-9.

Initial and boundary conditions

$$C(0,z) = C_s(0,z) = C_a(0,z) = 0$$

$$\overline{v}c_o = -D\frac{\partial C}{\partial z}\bigg|_{z=0} + \overline{v}C\bigg|_{z=0}$$

$$z \in [0..\infty)$$

$$\frac{\partial C(t, z \rightarrow \infty)}{\partial z} = 0$$

Method of solution

$$\boxed{A = \frac{M_r}{M_o}}$$

$$M_o = \int_0^{\omega} c_o(0\ \ ,t)\overline{v}d\omega\Big|_{\omega\to\infty}$$

$$M_r = \int_0^{\omega} f(z,t)d\omega\Big|_{\omega\to\infty}$$

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

$$\tilde{M_r} = \frac{\tilde{f}(z,s)}{s}$$

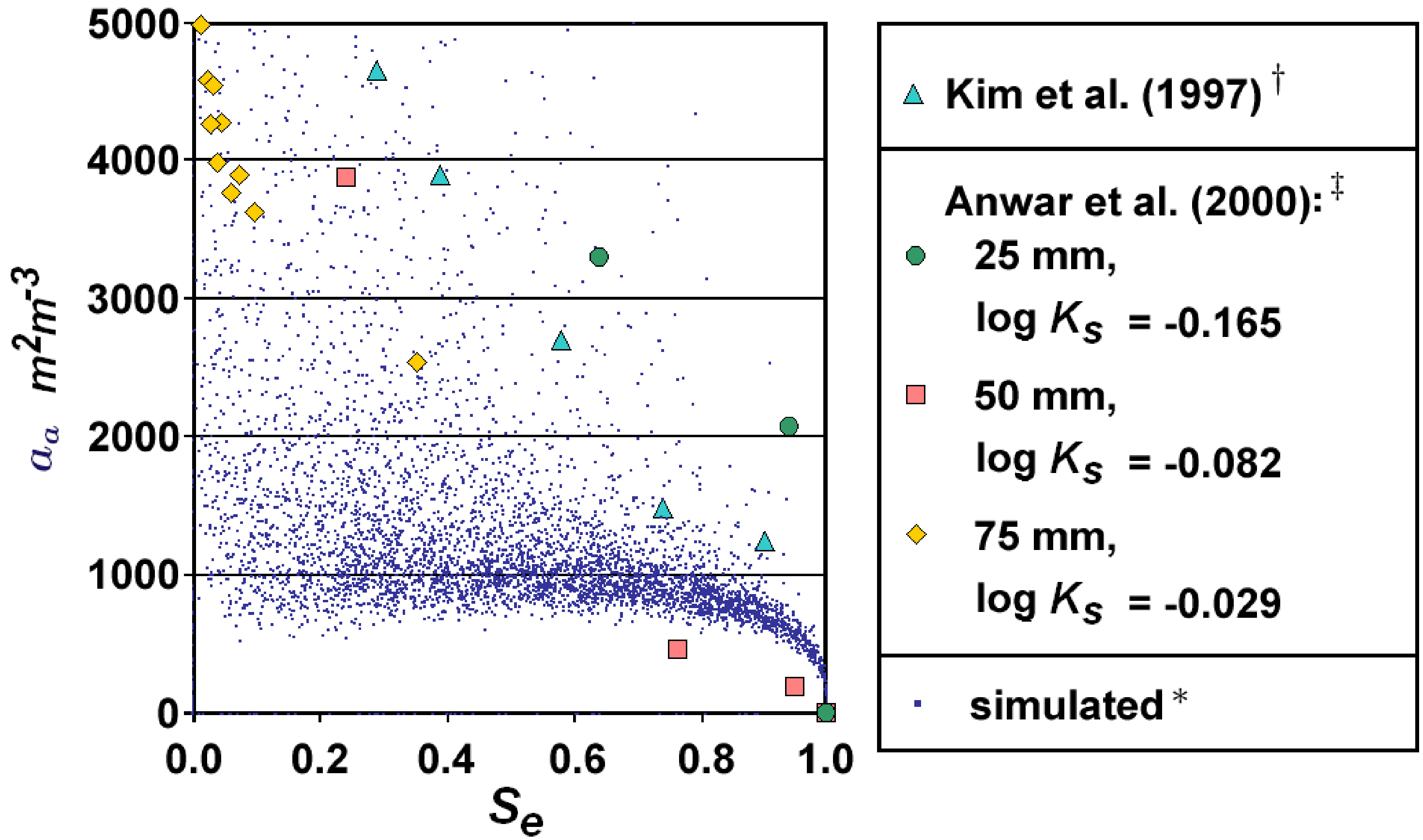
Air-water interfacial area

Rose and Bruce (1949)*

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

*Rose, W., Bruce, W.A, 1949. Evaluation of capillary character in petroleum reservoir rock. Trans Am Inst Metall Eng, 186:127-42.

Air-water interfacial area



†Kim H, Rao PSC, Annable MD. 1997 Determination of effective air-water interfacial area in partially-saturated porous media using surfactant adsorption, Water Resources Research 33(12):2705-11.

‡Anwar AHMF, Bettahar M, Matsubayashi U. 2000. A method for determining air-water interfacial area in variably saturated porous media. Journal of Contaminant Hydrology 43:129-46.

Database of soil parameter distributions

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

Soil*	Parameter	N	Mean	Standard Deviation	Units
sand	θ_r	308	0.050	0.003	L^3L^{-3}
	θ_s	308	0.367	0.032	L^3L^{-3}
	$\log_{10}K_s$	99¶	-0.691	0.218	$\log(m\ hr^{-1})$
	$\log_{10}\alpha$	308	0.5306	0.034	$\log(m^{-1})$
	$\log_{10}n$	308	0.482	0.077	$\log(dimensionless)$
	ρ	168¶	1.58×10^6	1.42×10^5	$g\ m^{-3}$
	r_p	0§	4.71×10^{-4}	1.60×10^{-5}	m
	α_z	1†	5.59×10^{-3}	0.00	m
	T	1944⋆	11.7	7.38	$^\circ\ Celsius$
silt loam	θ_r	330	0.063	0.013	L^3L^{-3}
	θ_s	330	0.406	0.050	L^3L^{-3}
	$\log_{10}K_s$	75¶	-2.160	-0.384	$\log(m\ hr^{-1})$
	$\log_{10}\alpha$	330	-0.207	0.075	$\log(m^{-1})$
	$\log_{10}n$	330	0.206	0.016	$\log(dimensionless)$
	ρ	133¶	1.43×10^6	1.48×10^5	$g\ m^{-3}$
	r_p	0§	1.18×10^{-4}	5.50×10^{-5}	m
	α_z	1‡	8.75×10^{-5}	0.00	m
	T	1944⋆	11.7	7.38	$^\circ\ Celsius$
clay	θ_r	84	0.101	0.011	L^3L^{-3}
	θ_s	84	0.515	0.085	L^3L^{-3}
	$\log_{10}K_s$	22¶	-2.085	0.0475	$\log(m\ hr^{-1})$
	$\log_{10}\alpha$	84	0.276	0.129	$\log(m^{-1})$
	$\log_{10}n$	84	0.114	0.015	$\log(dimensionless)$
	ρ	38¶	1.29×10^6	1.68×10^5	$g\ m^{-3}$
	r_p	0§	9.95×10^{-5}	6.15×10^{-5}	m
	α_z	1‡	8.75×10^{-5}	0.00	m
	T	1944⋆	11.7	7.38	$^\circ\ Celsius$

* Generated with the *Rosetta* program (Schaap et al. 1999). unless otherwise noted.
† Field lysimeter study by Poletika et al. (1995).
‡ Kaczmarek et al. (1997).
⋆ Data from *Remote Soil Temperature Network* [1].
¶ From the *UNSODA* database (Leij 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**

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

* 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 $\lambda^* \approx \lambda/2$.
§ Mazzone (1998) p. 114.

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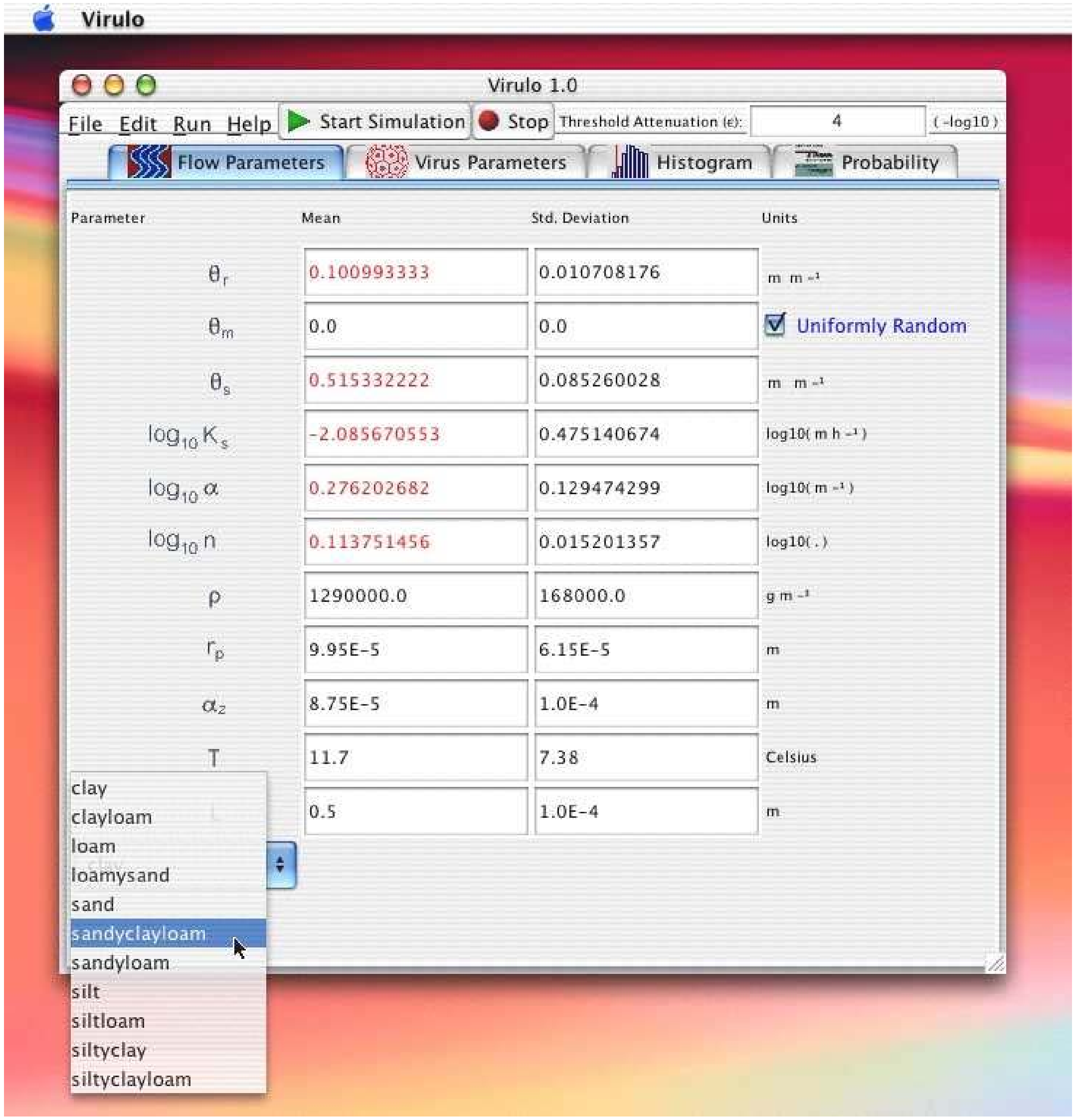
Virulo http://www.epa.gov/ada/



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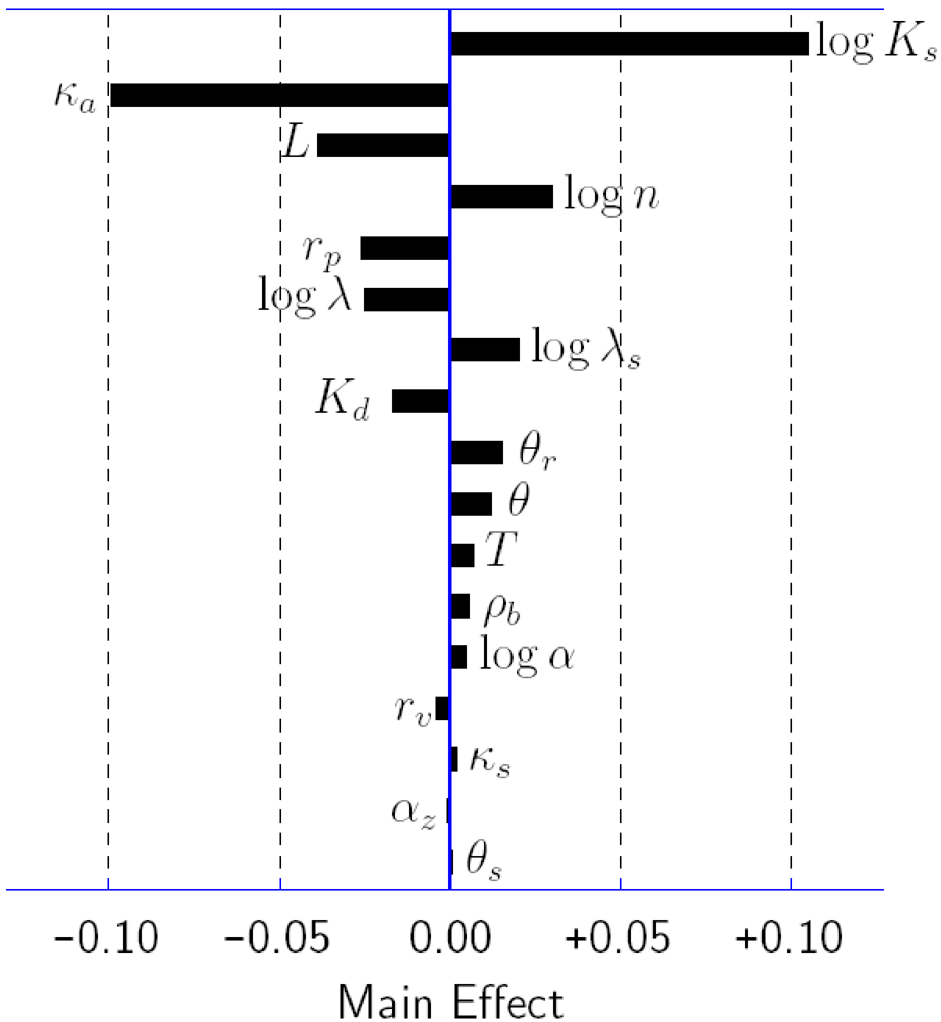
Results of sensitivity analyses



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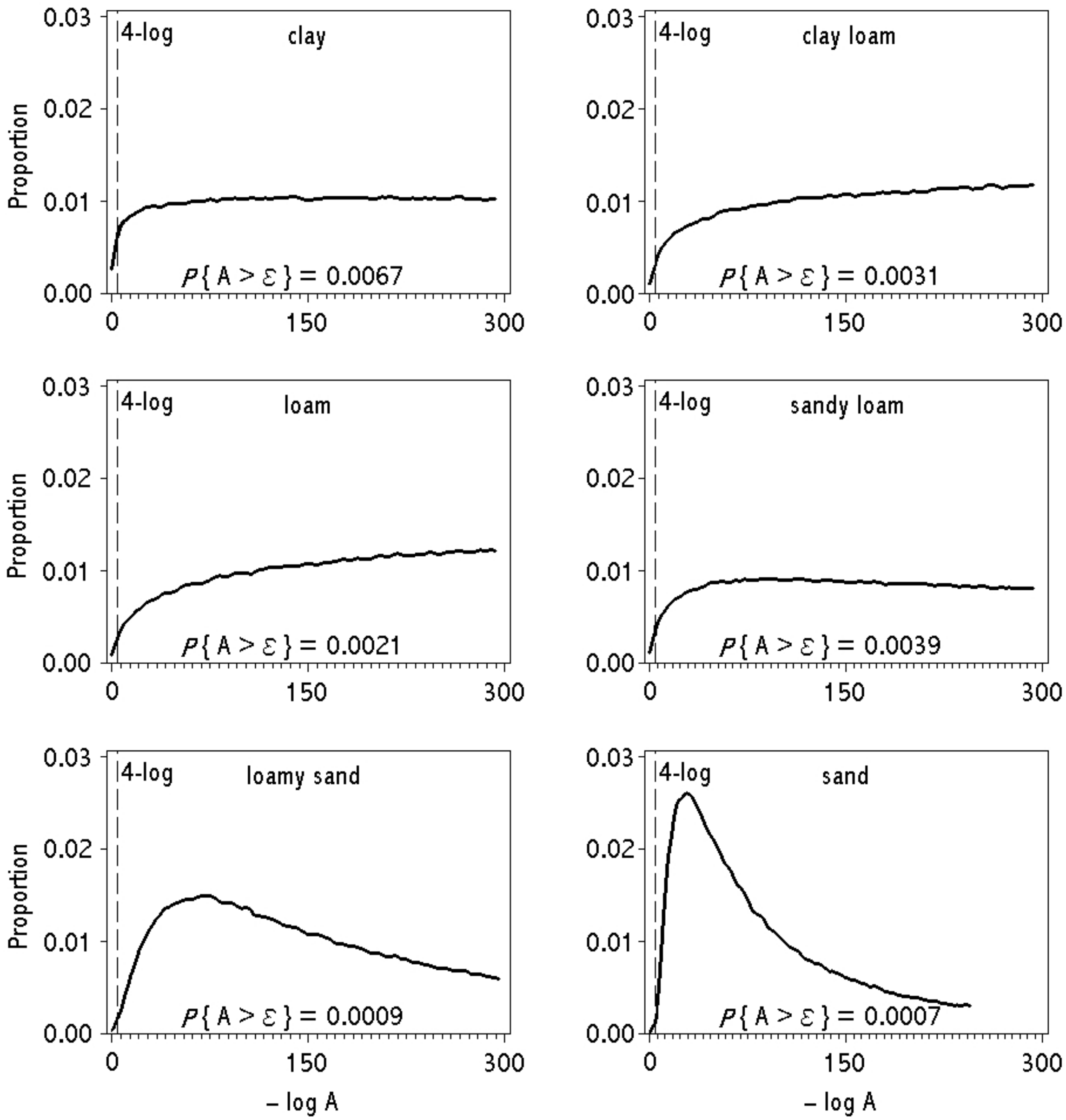
Results of Monte Carlo Simulations



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)

Faulkner BR, Lyon WG, Khan FA, Chattopadhyay S. 2003. Modeling leaching of viruses by the Monte Carlo method. Water Research (in press).