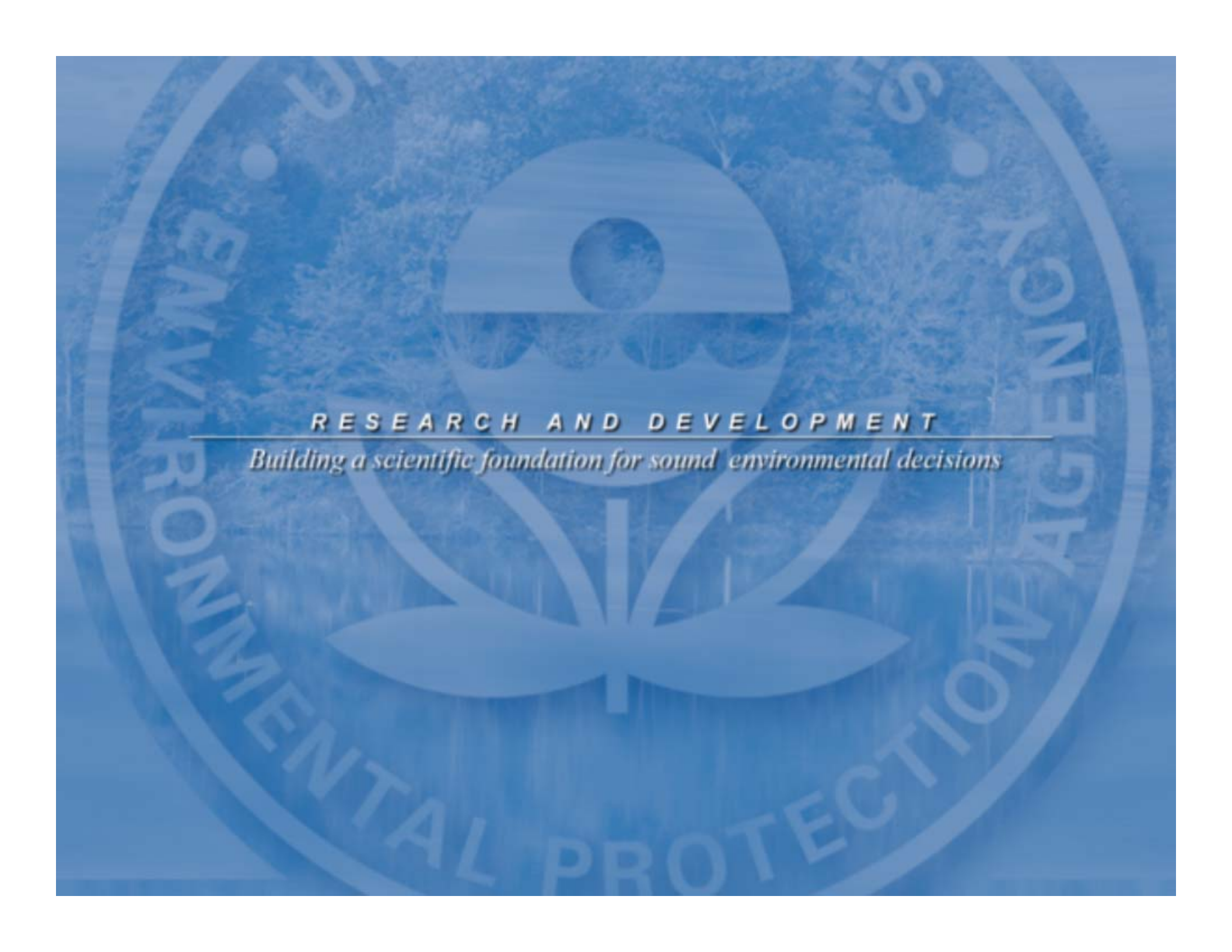


US EPA ARCHIVE DOCUMENT

The background of the slide features a large, semi-transparent watermark of the United States Environmental Protection Agency (EPA) logo. The logo is circular and contains a stylized flower with a globe as its center, surrounded by leaves. The words "U.S. ENVIRONMENTAL PROTECTION AGENCY" are written around the perimeter of the circle.

RESEARCH AND DEVELOPMENT

Building a scientific foundation for sound environmental decisions

One-Dimensional Variably Saturated Microbial Transport Simulations

Bart Faulkner

Hydrologist, ORD/NRMRL/GWERD

USGS/EPA STARS Grant Meeting on

Cryptosporidium Removal by Bank filtration

September 9 & 10, 2003

Collaborators

William Lyon, ManTech Env Research Services

Sandip Chattopadhyay, Battelle Columbus

Peter Breidenbach, ManTech Env Research Services

Faruque Khan, US EPA Headquarters

Jerome Cruz, Washington State Dept of Ecology

Outline

Modeling goals

Conceptual model

Governing equations and their solution

Monte Carlo Simulations and sensitivity analyses

Conclusions/Questions



RESEARCH &
DEVELOPMENT

*Building a
scientific
foundation
for sound
environmental
decisions*

Modeling Goals

Motivated by
Ground Water Rule:

Physically based

Probabilistic

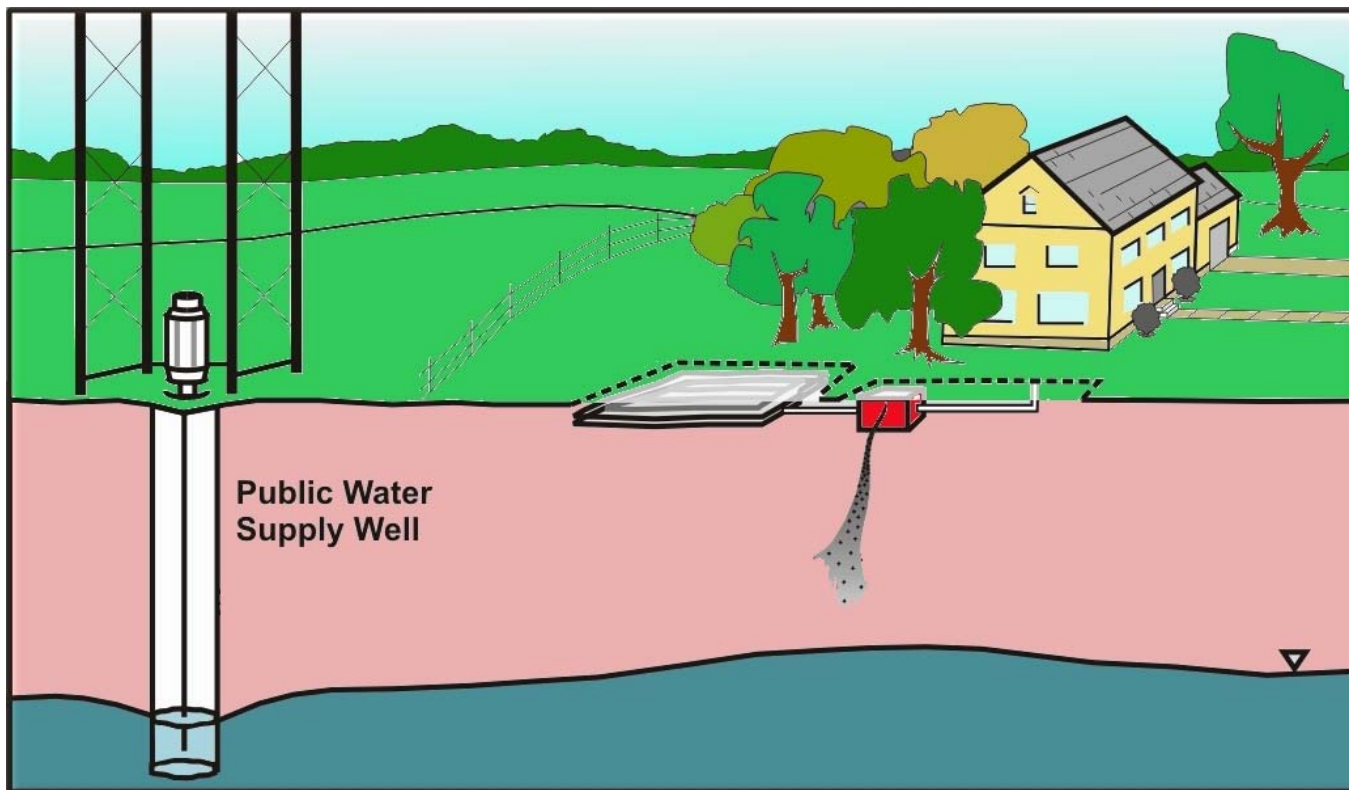


RESEARCH &
DEVELOPMENT

*Building a
scientific
foundation
for sound
environmental
decisions*

Modeling Goals

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

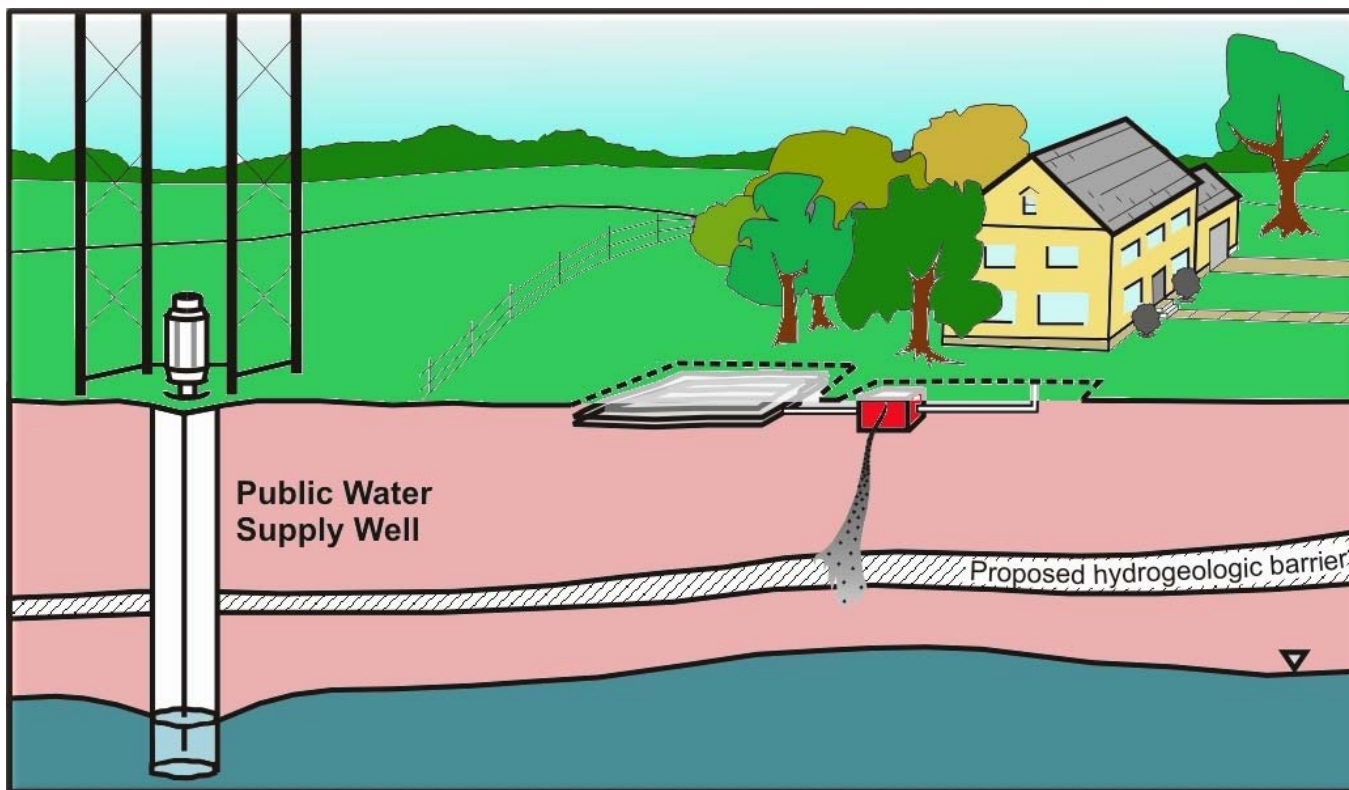


RESEARCH &
DEVELOPMENT

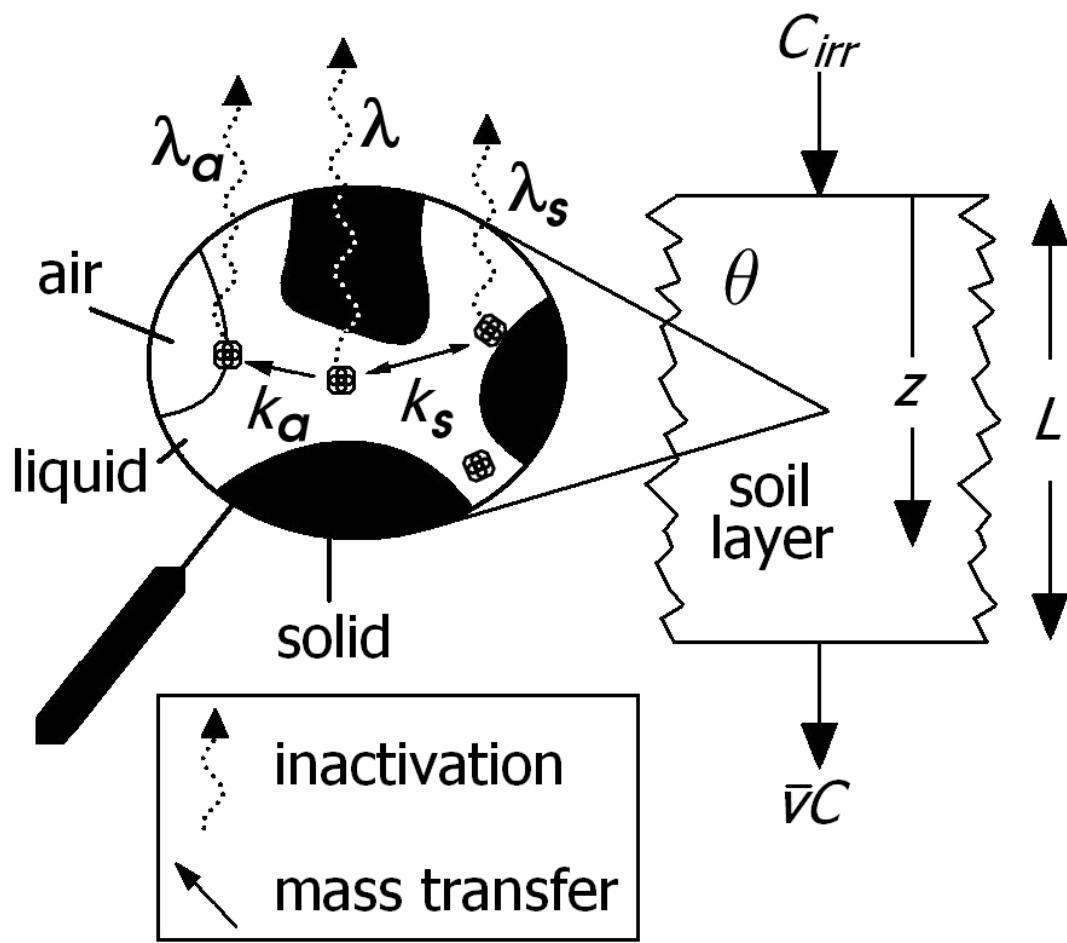
*Building a
scientific
foundation
for sound
environmental
decisions*

Modeling Goals

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



Conceptual model



Governing equations

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

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

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

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

Initial and boundary conditions

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

$$\bar{v}c_o = -D \left. \frac{\partial C}{\partial z} \right|_{z=0} + \bar{v}C \Big|_{z=0}$$

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

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

Method of solution

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

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

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

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

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

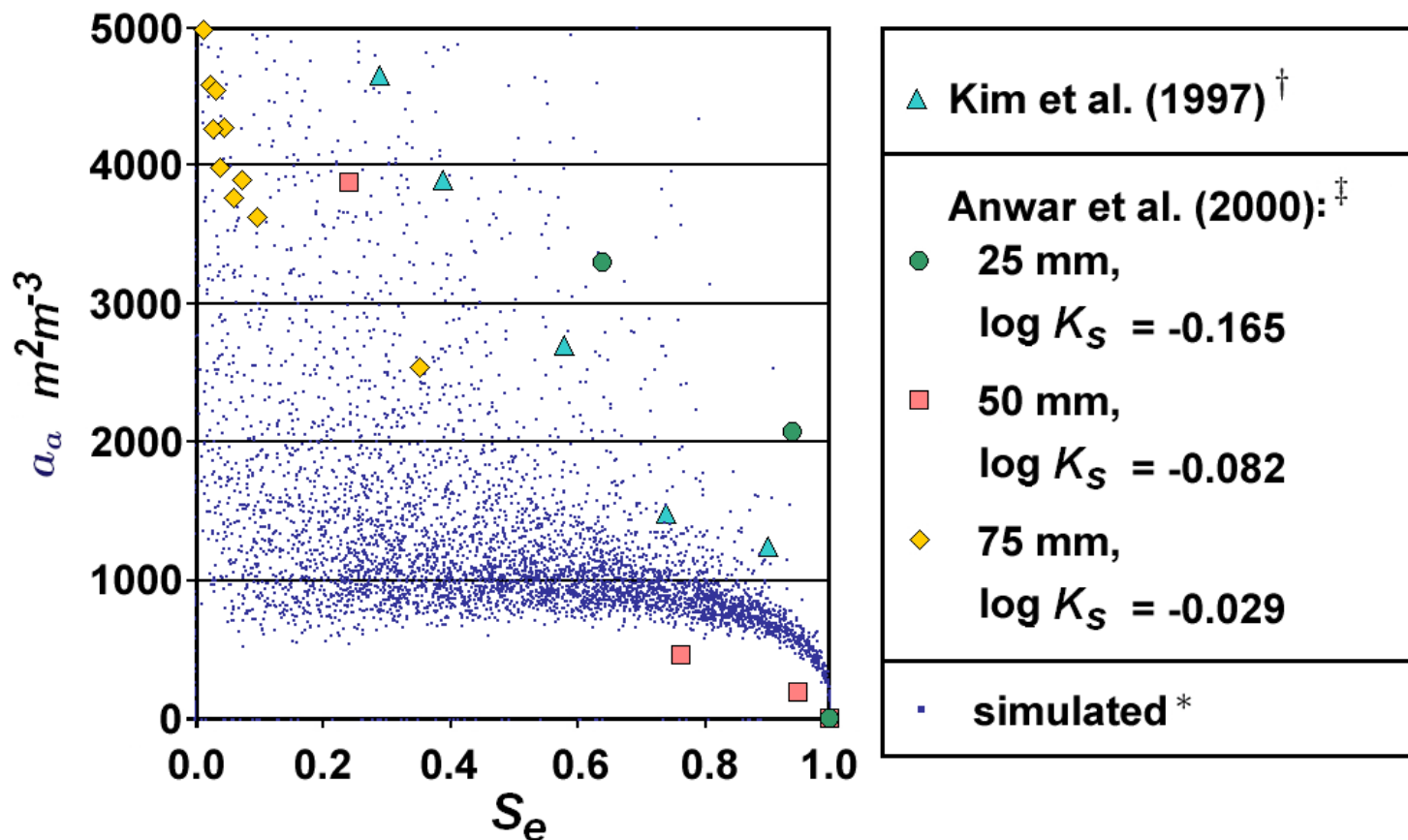
Air-water interfacial area

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	$\log(\text{dimensionless})$
	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	$\log(\text{dimensionless})$
	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	$\log(\text{dimensionless})$
	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}	$m hr^{-1}$
κ^\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 compiled 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.

RESEARCH & DEVELOPMENT

Building a scientific foundation for sound environmental decisions

Virulo

<http://www.epa.gov/ada/>

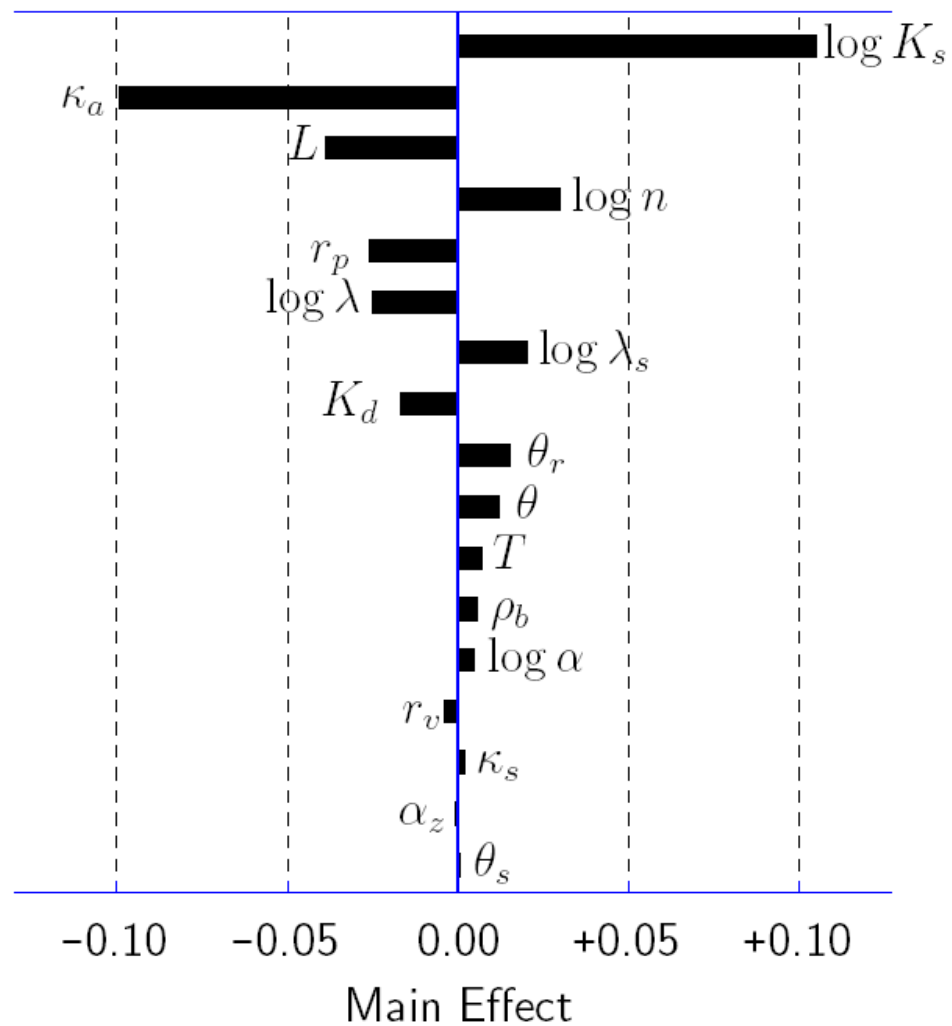
The screenshot shows the Virulo 1.0 software interface. At the top, there is a menu bar with 'File', 'Edit', 'Run', and 'Help'. Below the menu bar are buttons for 'Start Simulation' (a green play button) and 'Stop' (a red stop button). To the right of these buttons is a 'Threshold Attenuation (e):' field with the value '4' and a '(-log10)' label. Below the menu bar are four tabs: 'Flow Parameters', 'Virus Parameters', 'Histogram', and 'Probability'. The 'Virus Parameters' tab is currently selected.

The main window displays a table of parameters with the following columns: 'Parameter', 'Mean', 'Std. Deviation', and 'Units'. The parameters listed are:

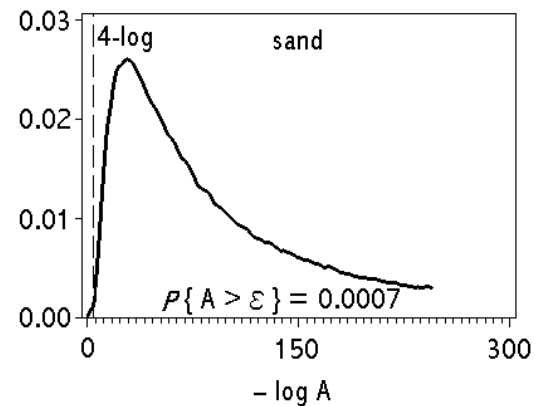
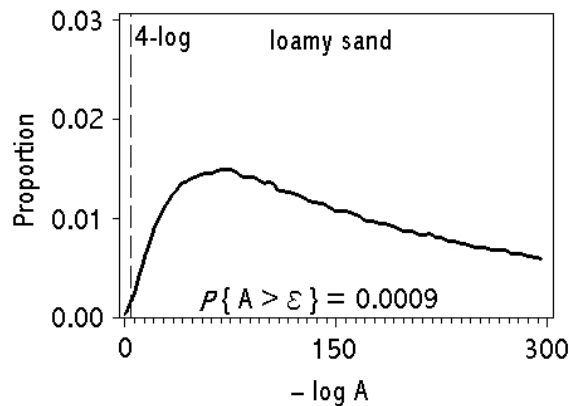
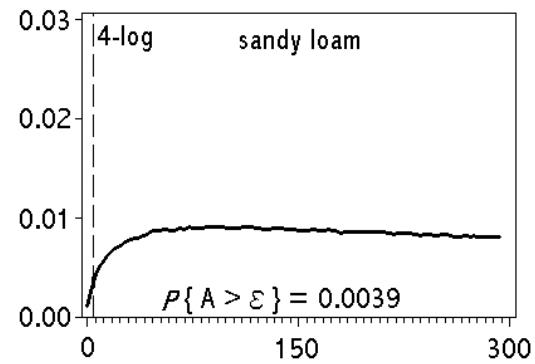
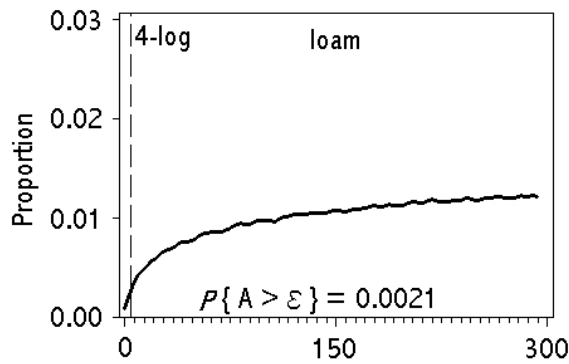
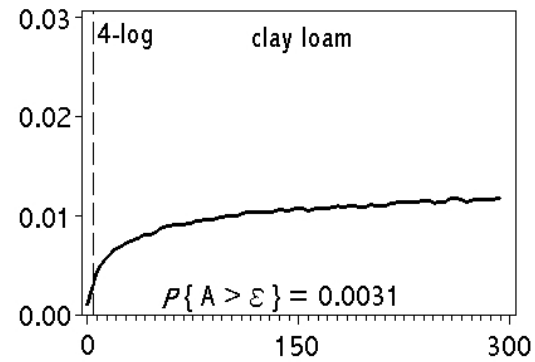
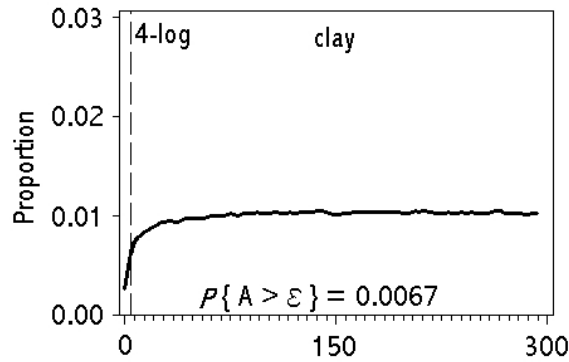
Parameter	Mean	Std. Deviation	Units
θ_r	0.100993333	0.010708176	m m ⁻¹
θ_m	0.0	0.0	<input checked="" type="checkbox"/> Uniformly Random
θ_s	0.515332222	0.085260028	m m ⁻¹
$\log_{10} K_s$	-2.085670553	0.475140674	log10(m h ⁻¹)
$\log_{10} \alpha$	0.276202682	0.129474299	log10(m ⁻¹)
$\log_{10} n$	0.113751456	0.015201357	log10(.)
ρ	1290000.0	168000.0	g m ⁻¹
r_p	9.95E-5	6.15E-5	m
α_z	8.75E-5	1.0E-4	m
T	11.7	7.38	Celsius
	0.5	1.0E-4	m

Below the table, there is a dropdown menu for soil types. The menu is open, showing the following options: clay, clayloam, loam, loamysand, sand, **sandyclayloam** (highlighted), sandyloam, silt, siltloam, siltyclay, and siltyclayloam.

Results of sensitivity analyses



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).