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Predicting Attenuation of Viruses During Percolation in Soils

2. User's Guide to the *Virulo 1.0 Computer Model*

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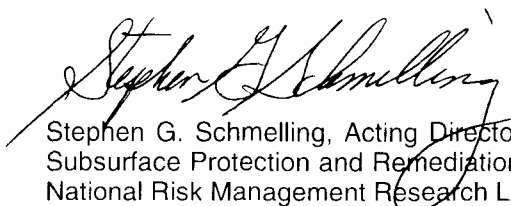
Foreword

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet this mandate, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for preventing and reducing risks from pollution that threatens human health and the environment. The focus of the Laboratory's research program is on methods and their cost-effectiveness for prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites, sediments and ground water; prevention and control of indoor air pollution; and restoration of ecosystems. NRMRL collaborates with both public and private sector partners to foster technologies that reduce the cost of compliance and to anticipate emerging problems. NRMRL's research provides solutions to environmental problems by: developing and promoting technologies that protect and improve the environment; advancing scientific and engineering information to support regulatory and policy decisions; and providing the technical support and information transfer to ensure implementation of environmental regulations and strategies at the national, state, and community levels

This publication has been produced as part of the Laboratory's strategic long-term research plan. It is published and made available by EPA's Office of Research and Development to assist the user community and to link researchers with their clients.

EPA's Office of Water is currently promulgating a Ground Water Rule to ensure water supplies are safe from contamination by viruses. States may be required to conduct hydrogeologic sensitivity assessments to predict whether a particular aquifer is vulnerable to pathogens. This work presents a User's Guide for *Virulo*, a user-friendly predictive screening model for virus attenuation above aquifers. It is hoped this model will be a useful tool for state regulators, utilities, and development planners.



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Abstract

In the EPA document *Predicting Attenuation of Viruses During Percolation in Soils 1. Probabilistic Model* the conceptual, theoretical, and mathematical foundations for a predictive screening model were presented. In this current volume we present a User's Guide for the computer model that implements the probabilistic model. The model is a predictive screening model called *Virulo*, so named because of its use of the Monte Carlo method for predicting virus fate and transport. This document presents a general overview of the parameters used and how they can be modified to suit a particular predictive modeling scenario. In addition, a non-technical overview of the conceptual modeling approach is given. Some example applications of *Virulo* are presented.

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Section 1. Introduction

Understanding the fate and transport of viruses and pathogens in variably saturated soil and aquifer materials is important in predicting potential risk to human health from human and animal wastes. The U.S. EPA Office of Water proposed the Ground Water Rule (U.S. EPA 2000), which will reduce exposure to pathogenic viruses and bacteria associated with human and animal wastes that might contaminate Public Water Supply wells. As part of the Ground Water Rule, public water supply systems that do not meet disinfectant treatment requirements will be required to conduct source water monitoring if the system produces water from sensitive aquifers¹.

The U.S. EPA Office of Research and Development has developed a virus fate and transport model (*Virulo*) that analyzes virus leaching from sorption sites in variably saturated soil and aquifer materials. *Virulo* predicts attenuation to total viruses as they pass through a soil layer. One use of the model could be to provide estimates of attenuation of viruses percolating through a candidate barrier layer of a particular soil textural type. However the model has many other potential uses such as predicting virus attenuation through land spreading of wastewater during ground-water recharge operations or for predicting the effects of high density septic tank discharge on ground-water quality.

1.1 What does *Virulo* do?

Virulo is a one-dimensional, variably saturated, ground-water flow and contaminant transport model. By computing analytical solution equations that describe advection, dispersion, viral sorption, inactivation, and mass transfer, ensembles of outputs are produced using random sampling of certain parameters over specified ranges and distributions through use of the Monte Carlo method

Virulo generates the number of cases in which a certain level² of virus attenuation was or was not achieved. As discussed in detail in *Predicting Attenuation of Viruses During Percolation in Soils. 1. Probabilistic Model* (hereafter referred to as "Part 1"), attenuation is defined as the ratio of total mass leaving the layer to the total mass entering it (Figure 1.1). Part 1 contains a detailed description of the system being modeled and the theoretical development of *Virulo*.

Virulo is a screening model only. It was developed to fill a niche for users who are expected to have only a small amount of information available for a site of interest. Default values, categorized by qualitative descriptions are emphasized. For more complete investigations of a site, numerical models such as *Viralt* (Park et al. 1992), *Virtus* (Yates et al. 1991), or *Canvas* (Park et al. 1991) should be considered. These models allow handling of heterogeneity, and other factors affecting transport and fate which are conceptually greatly simplified in *Virulo*.

1.2 What information is needed to run *Virulo*?

The transport component of the model primarily uses data from soil textural³ and thickness information (perhaps derived from boring logs) and soil survey reports for a particular site of interest. Human virus data at present are limited to polio, hepatitis A, reovirus 3, coxsackievirus, and echovirus.

Many parameters can be defaulted to standardized values on the input panels. Default parameters can also be overridden by the user when more accurate values are available for a particular site.

The default description of soil water content used internally is a climate-free estimate based on the assumption of a uniform random distribution of water content values chosen from values between the residual water saturation and complete water saturation for a given soil texture (Table 1.1). This distribution is used in the *Virulo* Monte Carlo calculations. The user currently has the option of overriding this distribution, and inserting a water content (e.g., the estimated field capacity or wilt point for the given soil texture) directly. This allows the user to gain a better appreciation for the effect of water content on virus breakthrough at the bottom of the soil layer of interest.

¹ Sensitive aquifers include karst, fractured bedrock, and gravel aquifers

² The targeted level of attenuation is adjustable by the user 4-log_{10} (99.99%) represents the current default level

³ The 12 USDA textural categories are used in *Virulo* to supply default parameters. See, for example, <http://www.agronomy.psu.edu/Courses/SOILS101/Labs/texture.html>.

Table 1.1 Summary of Notation Used in the Virulo Input Data Windows

Parameter	Description	Units
Flow Parameters Window (given in sequence):		
θ_r	Residual water content, the water content that is approached at highly negative capillary pressure, where the water remaining is that held by the soil's capillary forces	$m^3 m^{-3}$
θ_m	Water content, the volume fraction containing water	$m^3 m^{-3}$
θ_s	Saturated water content, equal to the porosity	$m^3 m^{-3}$
$\log_{10}(K_s)$	Saturated hydraulic conductivity, the hydraulic conductivity the soil would have if $\theta_m = \theta_s$	$\log_{10}(m h^{-1})$
$\log_{10}(\alpha)$	van Genuchten parameter [†]	$\log_{10}(m^{-1})$
$\log_{10}(n)$	van Genuchten parameter [†]	\log_{10}
ρ	Soil dry bulk density	$g m^{-3}$
r_p	Mean soil particle radius	m
α_z	Hydrodynamic dispersivity	m
T	Mean soil temperature, used for computing molecular dispersivity of the virus, a component of dispersion	°C
L	Thickness of candidate barrier layer	m
Virus Parameters Window (given in sequence)		
β	Exponential decay exponent in source term	h^{-1}
$\log_{10}(\lambda)$	Mobile virus inactivation rate constant, rate of inactivation of suspended viruses	$\log_{10}(h^{-1})$
$\log_{10}(\lambda^*)$	Solid-sorbed virus inactivation rate constant, rate of inactivation of soil-adsorbed viruses	$\log_{10}(h^{-1})$
κ	Mass transfer coefficient, mobile phase to solid-sorbed phase [†]	$m h^{-1}$
κ	Mass transfer coefficient, mobile phase to air-water interface sorbed [‡]	$m h^{-1}$
r_v	Mean virus radius	m
C_{max}	Maximum virus concentration in source term, arbitrary units	[e.g , PFU L ⁻¹]
K_d	Equilibrium partitioning coefficient for viruses sorbing onto soil particles	$m^3 g^{-1}$

*the van Genuchten relation is $\left(\frac{\theta_m - \theta_r}{\theta_s - \theta_r}\right) = \frac{1}{\left[1 + (\alpha h)^n\right]^m}$, $m = 1 - \frac{1}{n}$

†the rate itself is computed in *Virulo* by $k = \kappa a_T$ where a_T is the water-solid interfacial area.

‡the rate itself is computed in *Virulo* by $k^\diamond = \kappa^\diamond a_T^\diamond$ where a_T^\diamond is the water-air interfacial area.

Figure 1.1 shows schematically, at the microscopic level, the interaction among the various parameters, and the descriptions of their physical basis are also described in detail in Part 1.

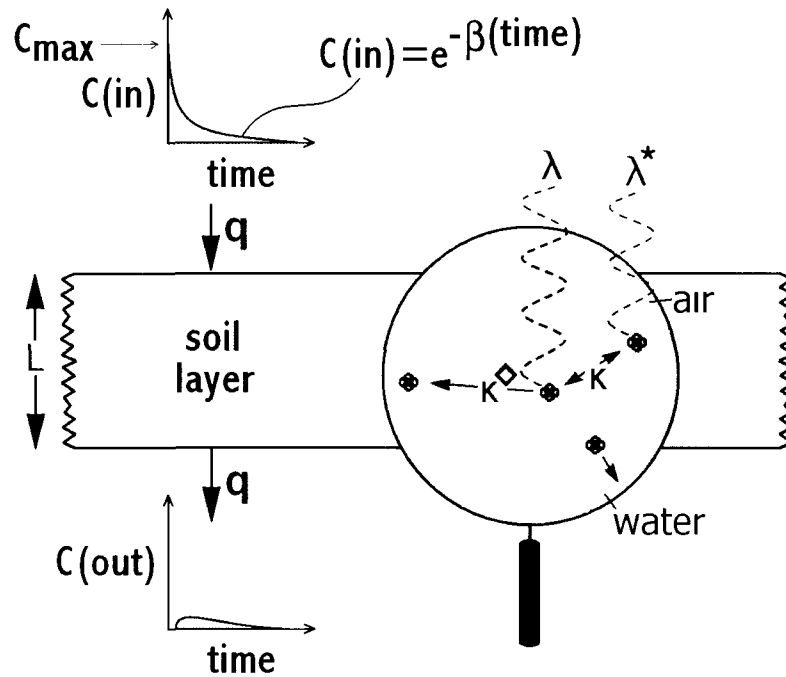


Figure 1.1 Schematic depiction of physical role of microscopic parameters discussed in detail in *Predicting Attenuation of Viruses During Percolation in Soils. 1. Probabilistic Model.*

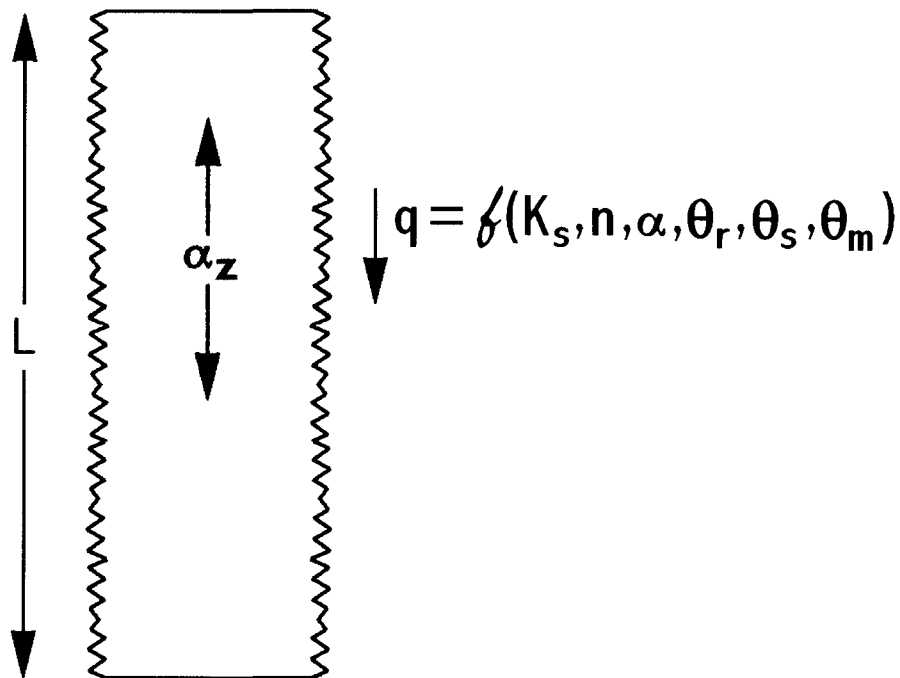


Figure 1.2 Schematic depiction of physical role of macroscopic parameters discussed in detail in *Predicting Attenuation of Viruses During Percolation in Soils. 1. Probabilistic Model.*

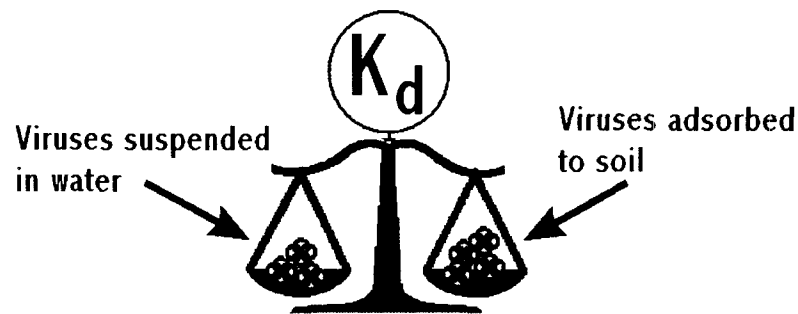


Figure 1.2 shows the macroscopic parameters that describe advective flux and dispersion of viruses as they pass through the soil layer of interest. Figure 1.3 illustrates the role of K_d , the equilibrium partitioning coefficient.

Figure 1.3 Schematic depiction of physical role of the equilibrium partitioning coefficient, discussed in detail in *Predicting Attenuation of Viruses During Percolation in Soils. 1. Probabilistic Model.*

Virulo makes use of a conceptual model that simplifies the types and rates of natural processes that govern variably saturated ground water flow and virus transport. As noted in Part 1, *Virulo* employs the following simplifications and assumptions:

- One-dimensional, vertical, uniform, variably saturated, ground-water flow
- Gravity drainage only (no abrupt change in capillary pressure in the soil)
- Random soil water content representing random, instantaneous recharge from precipitation
- There is no soil water hysteresis and water content is random, rather than cyclical, wetting and drying (the results are very sensitive to the water content)
- Variably saturated ground-water flow through uniform layers of porous media without preferential flow pathways
- Virus transport may be simulated by linear sorption typical of dissolved contaminants rather than by colloidal filtration theory specific to colloidal particles
- Measured laboratory, rather than field, values of virus transport and survival are suitable for use in the simulations
- Parameter values are displayed with significant figures not warranted by the actual measurements available to the user to allow use of a variety of data sources with varying significant figures. The user should recognize that the results are suitable for informational purposes only; i.e., four log removal could be undistinguishable from two log removal or six log removal given available data and theory

The figures are merely meant to illustrate the role of the parameters used in *Virulo*. For a complete description of the processes they represent, Part 1 should be studied.

In order to quantify uncertainty in model outputs, *Virulo* employs the Monte Carlo method (Figure 1.4). The method works in *Virulo* by assuming the values of the parameters vary randomly in one of two possible ways:

- the input parameters vary randomly and independently of each other, but they follow a normal distribution described by the mean and standard deviation; or,
- the input parameters vary randomly, but dependently with a subset of the other parameters, and they follow a multivariate normal distribution described by their means and their variance-covariance matrix.

The parameters in *Virulo* which vary according to the latter are the hydraulic parameters θ_r , θ_s , $\log_{10} K_s$, $\log_{10} a$, $\log_{10} n$. This is important to the user because their standard deviations cannot be modified because *Virulo* employs the variance-covariance matrix, computed a priori for each of the twelve USDA soil types. The current version does not allow the user to modify the underlying matrix used in the dependent *conditional* simulations for these input parameters. Furthermore, modifying the mean values of these five parameters is not recommended because it is dubious to assume the variance-covariance matrix would remain unchanged, and presumably the greater the magnitude of the adjustment in the mean, the greater the error in the existing variance-covariance matrix. The user

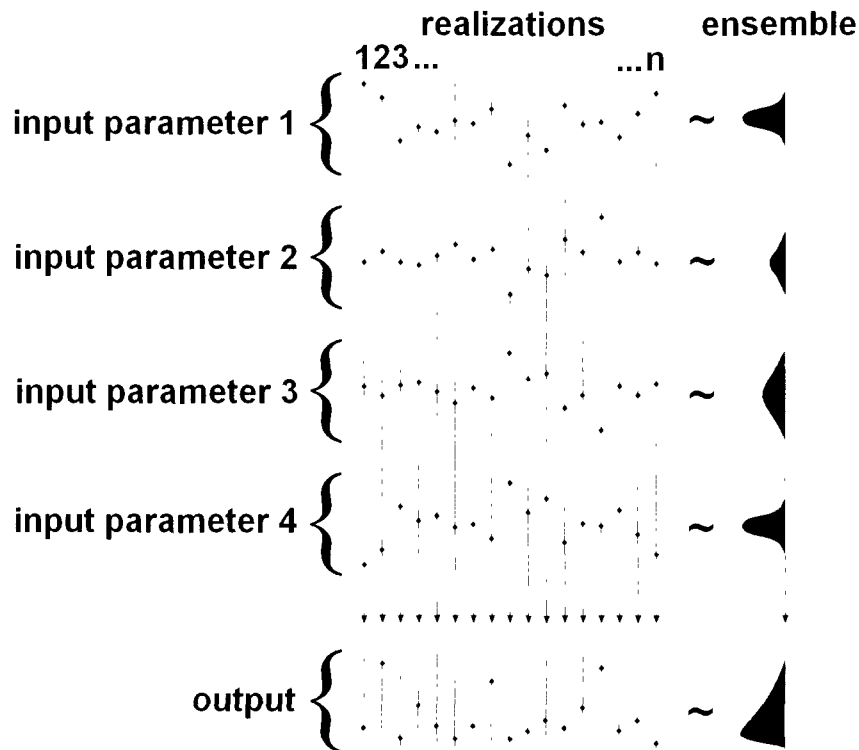


Figure 1.4 Schematic depiction of how the Monte Carlo method works. Each realization is a random sample of input parameters. The collection of all realizations is the ensemble, from which inference is made on the output.

is advised not to change these values unless they have a complete understanding of the way conditional dependence is simulated in *Virulo*, as described in Part 1, and they are completely able to justify the change made.

The Monte Carlo method uses computer-generated random numbers. In models such as *Virulo*, the Monte Carlo method works as follows:

- I. A randomly generated set of input parameters is created and the model is run to produce an output.
- II. Step I is repeated many times, building up a list of output values corresponding to each random set of input parameters.
- III. After suitably many such runs (enough runs so that the user is confident the full range of possible inputs has been covered), inference is made on the output.

In the case of *Virulo*, the outputs (attenuation values) are plotted on a logarithmic scale as a right-truncated histogram. The user is free to adjust any of the parameters provided they can justify doing so. Furthermore, a user may wish to run *Virulo* by assuming one or more of the parameters is deterministic (i.e., does not vary). This is done by simply setting the standard deviation for the parameter to zero. Note that some of the parameters are given as the \log_{10} of its value. This is because these parameters are either known to follow, or are thought to follow the lognormal distribution, hence the user should be careful to note this if the values are adjusted from the defaults.

In addition to the special case of the conditional dependence of some of the input parameters, another special case should be discussed here: The value of the water content will depend not only on soil type, but on many external factors, such as climate, time of year, presence of irrigation, and evapotranspiration. Indeed, for most sites users will not have definitive information about its value. Therefore, *Virulo* offers two ways to model its value:

- it varies in a uniformly random manner between the residual water content at the lower end, and the saturated water content at the upper end (this is the default);
- the user can input a value and a standard deviation, as is done with the other independent parameters.

As is discussed in Part 1, the parameters to which the output is most sensitive are the hydraulic parameters. This may be viewed as fortunate, because these parameters and their variation are better studied and documented at present, than the parameters directly related to microscopic adsorption and decay.

Section 2. The *Virulo* User Interface

The main data input windows for *Virulo* consist of two panels, one denoted “Flow Parameters,” and one denoted “Virus Parameters.” These two panels are displayed on the following two pages as Figures 2.1 and 2.2. Despite the names, both panels contain some parameters that straddle more than one category. For example, the Flow Parameters panel contains some soil parameters, and the Virus Parameters panel contains some virus properties that are specifically for a certain soil texture. Nevertheless, the rough subdivision into two panels clusters together parameters controlling flow, and parameters controlling virus inactivation and sorption.

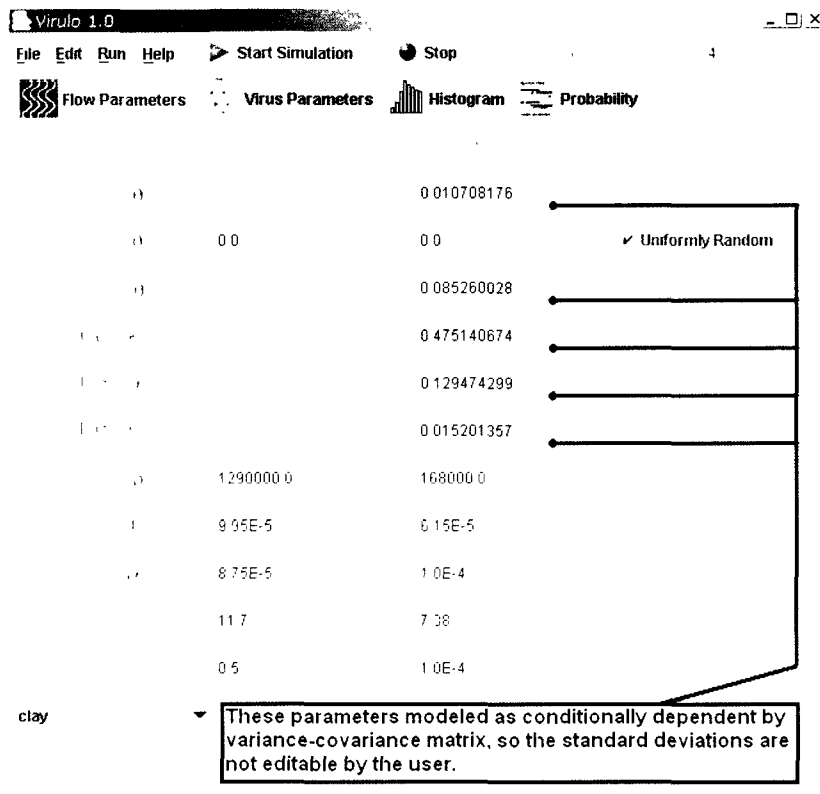


Figure 2.1 Default flow parameters upon first opening *Virulo* (Windows™ Version).

The input variables are denoted by symbols, which reflect common usage in the published literature. In case of doubt, resting the cursor on the symbol opens an identity box, which gives a short description of the variable denoted by the symbol.

When first opened, *Virulo* has default values corresponding to clay, and polio-clay entered for each of the parameters, and for the standard deviation to be associated with the parameter values. On the far right side, the dimensions for the entered parameter are indicated. In order to run *Virulo*, appropriate values for the parameters expressed in the necessary units must be entered in each of the active boxes. This can be accomplished in one of two ways

Method One is simply the use of the built-in default options as they stand. At the bottom of each panel is a box that activates a pull-down list of default options for a given soil texture, selection of which will automatically fill in all the appropriate parameters. This makes the program very easy to run for simple cases.

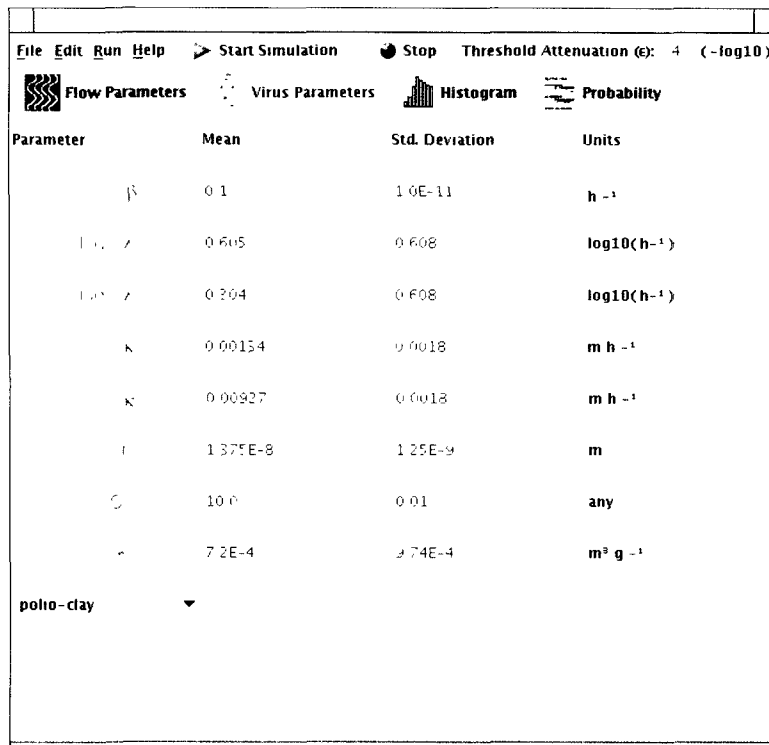


Figure 2.2 Default virus parameters upon first opening *Virulo* (Linux (WindowMaker) Version).

Method Two involves the more laborious filling in of the parameters one by one based on a detailed knowledge of the site. These parameters might be obtained independently (see Schijven and Hassanizadeh, 2000), from the compilation of Breidenbach et al., 2000⁴. **Great care must be taken to convert all parameters into the exact units specified by the input panel.**

Finally, we should mention that Methods One and Two can be combined. Method One can be used to fill in most of the parameters, leaving only a few parameters to be changed to fit the particular situation prevailing on the site of interest. The parameters can be changed repeatedly, and are not finalized until the program is actually run.

Note that in Figure 2.1 the "uniformly random" box opposite θ_m has been checked as the default. If this box is unchecked, then the θ_m parameter and its standard deviation may be edited. Various water contents consistent with the values of θ_s and θ_m may be inserted here, e.g., values for the field capacity and wilt point for the given texture. It is recommended that the standard deviation be kept very small (e.g., 0.001) for benchmark calculations of this type.

The value of the threshold attenuation can be set by the user by typing it in the text field at the right side of the toolbar of the main window frame. This is the level of attenuation being considered. Attenuation less than this value is considered an *exceedance* for that particular Monte Carlo run. In this way the user can set what constitutes an exceedance, for their purposes. A vertical red bar will be displayed in the histogram panel indicating the threshold attenuation chosen. By default, this value is set to 4, indicating a threshold of "4-log attenuation." This value is often mentioned in the context of proposed hydrogeologic sensitivity assessments, as well as in Comprehensive Performance Evaluations for public water systems. In the future, such performance evaluations will consider ground-water systems. The value is completely arbitrary, and is offered as a way for the user to make judgments or inferences from the model runs.

2.1 Soil and Flow Parameters

In the following Figure 2.3, the flow input panel is shown with the pull-down list of default textures. The clay default option was selected, and the program has inserted all the appropriate parameters for an "average" clay. The basis for selecting these default values is given in Faulkner et al., 2002.

The user will notice that when the model is running on their computer some of the parameter values are highlighted in red, some in regular black and white, and some of the standard deviations are grayed-out. Holding the cursor on any red-highlighted value will produce a message box indicating that "Modifying this mean value is not recommended. See model

⁴ We anticipate making a data compilation available in the future as a separate document

documentation.” Study has shown that the model results are highly sensitive to these red-highlighted parameters. The grayed-out standard deviations indicate that these values cannot be changed. Only those parameters and standard deviations appearing in regular black and white should ordinarily be changed.

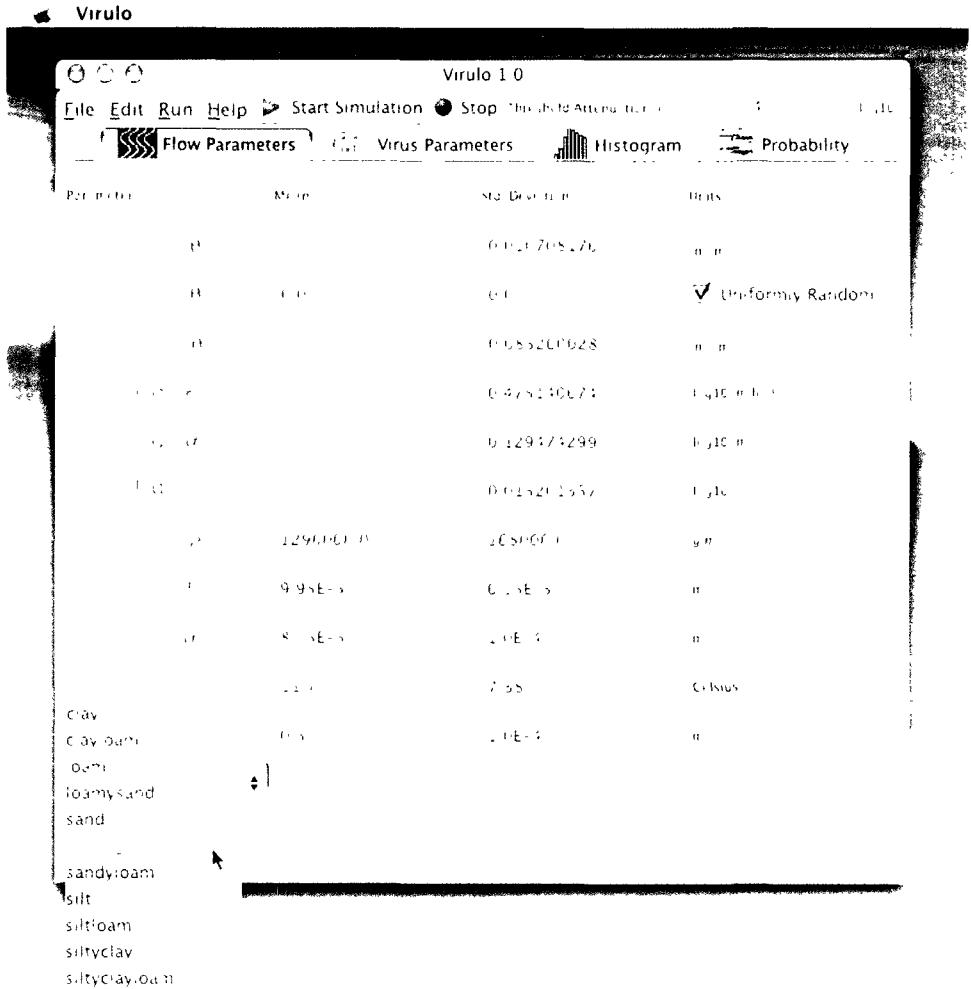


Figure 2.3 Flow input panel showing pull-down list of soil textures (Mac OS X Version)

2.2 Virus Parameters

In the following Figure 2.4, the virus input panel is shown with the pull-down list of virus and soil textures. The polio-clay default option was selected, and the program has inserted all the appropriate parameters for an “average” clay. The basis for selecting these default values as well as guidance for selecting custom values for a real site are given in Breidenbach et al., 2000.

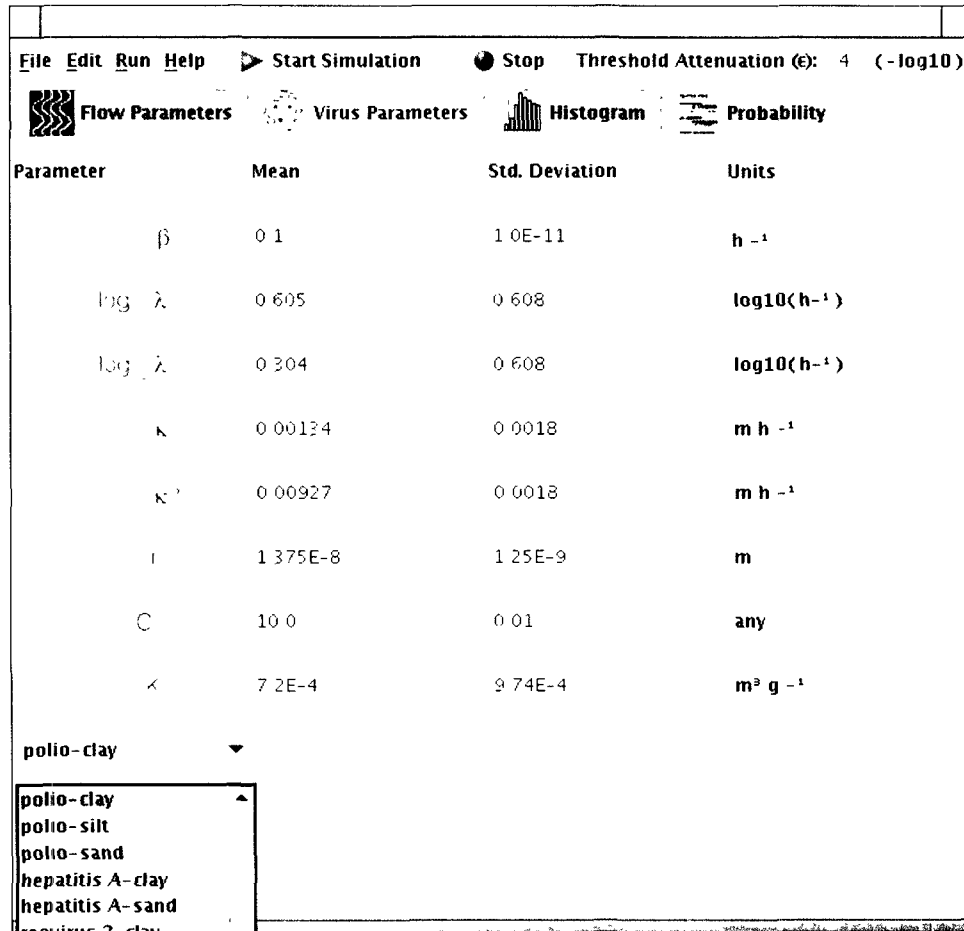


Figure 2.4 Virus input panel showing pull-down list of virus-texture defaults (Linux (WindowMaker) Version).

Section 3. Example Applications

Following entry of the default clay parameters, and the default polio-clay parameters, one can proceed to run the simulation. Figure 3.1 displays how the simulation is set to run, just after selection of the virus parameters. One can also proceed by clicking on the green arrow button. Typical run times are approximately 3 minutes⁵.

The simulation generates two kinds of output. The graphical histogram output, which is displayed continuously developing during the simulation, is shown below in final form as Figure 3.2. The vertical red bar separates cases of failure to attenuate (left of the bar) from successfully attenuated cases (right of the bar). The horizontal axis is the negative base-10 logarithm of the attenuation (A). The negative is used merely to allow the user to intuitively view increasing attenuation to the right, decreasing attenuation to the left. In the simulation shown, zero cases of failure were calculated in 10^6 iterations; thus, the probability of failure to achieve 4-log_{10} attenuation of poliovirus under all the prevailing assumptions about texture, water content, etc. is very low. If it were necessary to estimate this probability more precisely, further simulations could be run and accumulated until several cases of failure were seen. This is done by checking the *Retain and Accumulate* box on the histogram panel. When this box is checked, results from the simulation are included in the next simulation. This can be done as many times as needed in order to produce an acceptable histogram of outputs

Probability Output as text can also be obtained by clicking on the appropriate tab. The output contains a complete list of all parameter values assumed in the simulation. This text information can readily be clip-boarded into another program for formatting and printing. Below we display this text output information (edited to manuscript format) for the clay, polio-clay simulation, and random water content:

Output from *Virulo* Model:

Input parameters used:

Parameter: Mean Value(Standard Deviation) units:

Soil Parameters:

Residual water content: 0.1(0.01) $\text{m}^3 \text{m}^{-3}$

Water content: random between Residual water content and Saturated water content.

Saturated water content: 0.52(0.09) $\text{m}^3 \text{m}^{-3}$

Hydrodynamic dispersivity: $8.75\text{E-}5(1.0\text{E-}4)$ m

Log van Genuchten's alpha: 0.28(0.13) $\log_{10}(\text{m}^{-1})$

Log van Genuchten's n: 0.11(0.02) $\log_{10}(\cdot)$

Temperature of soil (for computing molecular diffusivity): 11.7(7.38) Celsius

Soil bulk density: 1290000.0(168000.0) g m^{-3}

Mean soil particle radius: $9.95\text{E-}5(6.15\text{E-}5)$ m

Log Saturated hydraulic conductivity: -2.09(0.48) $\log_{10}(\text{m h}^{-1})$

Thickness of proposed barrier: 0.5(0.1) m

Virus Parameters:

Coefficient of exponential decay of input concentration: 0.1(1.0E-11) h^{-1}

Log Mobile Virus Inactivation Rate: 0.605(0.608) $\log_{10}(\text{h}^{-1})$

Log Solid-sorbed Virus Inactivation Rate: 0.304(0.608) $\log_{10}(\text{h}^{-1})$

⁵ For the example above, run times were typically 2 minutes 43 seconds for 10^6 iterations on a Pentium III system with 128 Mb RAM operating under Windows98, and no other programs running concurrently

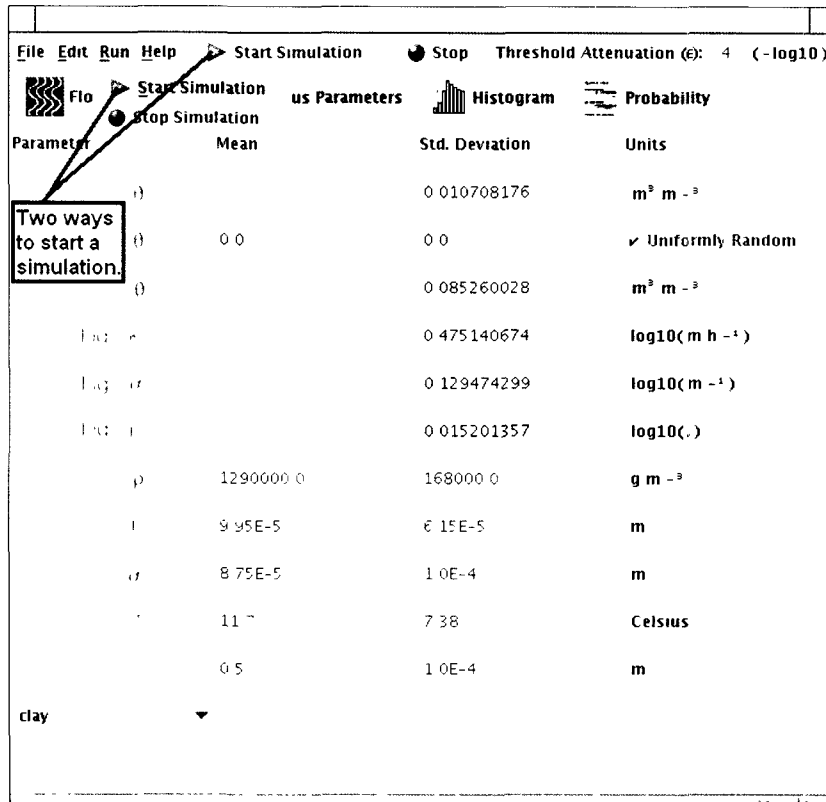


Figure 3.1 Virus property panel showing start of simulation (Linux (WindowMaker) Version).

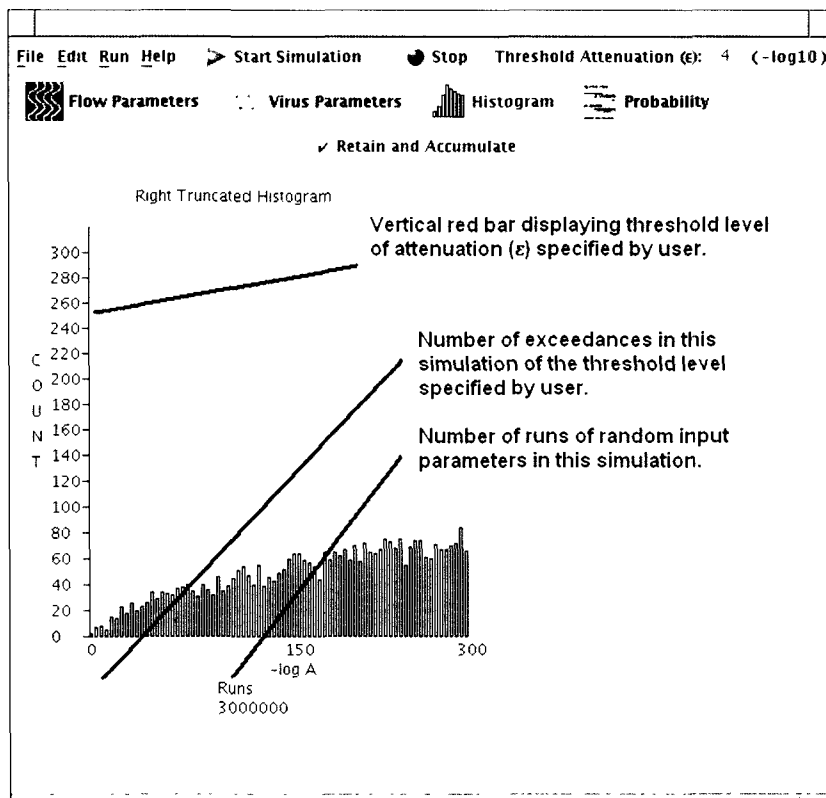


Figure 3.2 Histogram for a single simulation of default case Clay, Polio (Linux (WindowMaker) Version).

Mobile to solid-sorbed mass transfer coeff : 0.00134(0.0018) m h⁻¹
 Mobile to air-sorbed mass transfer coeff.: 0.00927(0.0018) m h⁻¹
 Radius of virus: 1.375E-8(1.25E-9) m
 Maximum virus concentration entering proposed barrier: 10.0(0.01) any
 Mobile to solid-sorbed equilibrium partition coeff.: 7.2E-4(9.74E-4) m³ g⁻¹

The probability of failure to achieve 4.0-log attenuation from 1000000 Monte Carlo runs was 0:1000000

The last entry gives the probability of failure to achieve successful reduction of virus concentration. In the computed case, this is apparently a relatively low probability⁶, and such a clay barrier would, therefore, under the assumed moisture conditions seem fairly adequate to prevent poliovirus contamination of an aquifer beneath it.

Figure 3.3 shows the histogram result for a default loamy sand with hepatitis A, K_d value for clays. In this case the histogram shows a distinct mode in the neighborhood of 60-log attenuation. By observing the shape of the histogram the user can obtain information about the distribution of attenuation values and how they behave in the vicinity of the chosen threshold attenuation. The maximum of 300-log is close to the numerical double precision limit of most modern math processors.

Figure 3.4 shows the output for hepatitis A with a default sandy loam soil. However, in this case the volumetric water content was set to 0.2, with a standard deviation of 0.05, instead of varying in a uniformly random way. It shows the dramatically different results that can be obtained if information is known about the water content. In this case the mode is very close to zero, and the probability of failure is very high

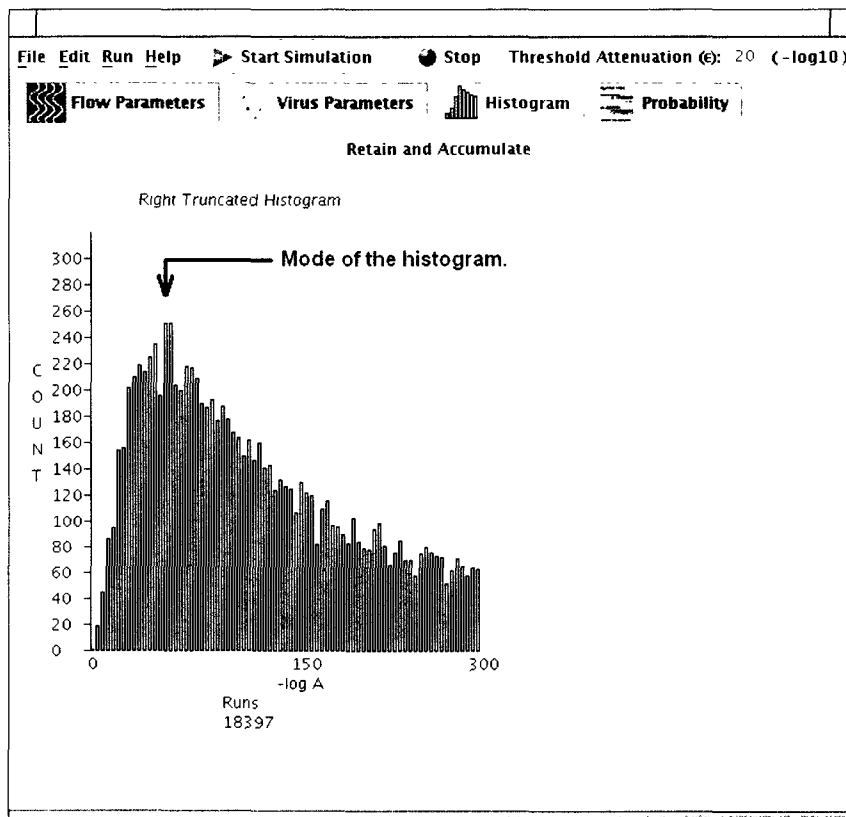


Figure 3.3 Histogram for a single simulation of default loamy sand, hepatitis A-Clay (Linux (WindowMaker) Version).

⁶ Further accumulated simulations yielded ca 1 chance in 1.2 million. Note that Virulo offers no guidance regarding what constitutes an "acceptable risk" in any given case. This judgment requires additional considerations well beyond the scope of the simple transport model described here.

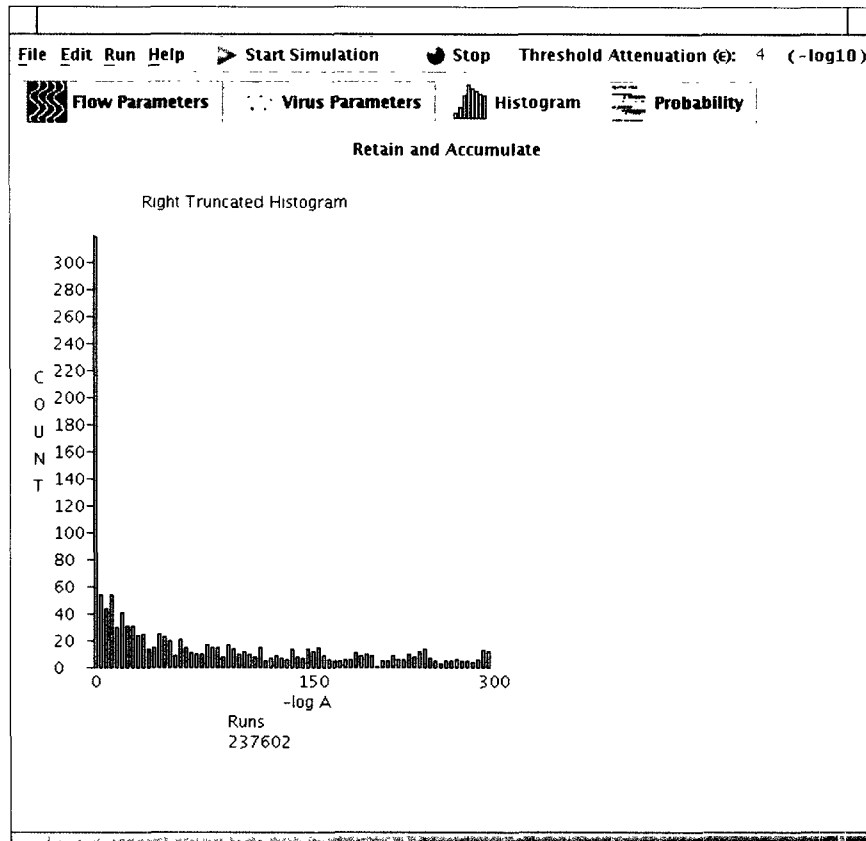


Figure 3.4 Histogram for a single simulation of default sandy loam with θ_m mean set to 0.2 and its standard deviation set to 0.05, hepatitis A-Clay (Linux (WindowMaker) Version).

To estimate the ability of a clay layer to attenuate poliovirus under wetter conditions, the simulation was run with the water content set to the approximate field capacity of clay⁷.

Further Output from *Virulo* Model with $\theta_m = \text{Field Capacity}$

Input parameters used:

Parameter: Mean Value(Standard Deviation) units:

Soil Parameters:

Log van Genuchten's alpha: 0.28(0.13) $\log_{10}(\text{m}^{-1})$

Residual water content: 0.1(0.01) $\text{m}^3 \text{m}^{-3}$

Water content: 0.47 (0.00) $\text{m}^3 \text{m}^{-3}$

Saturated water content: 0.52(0.09) $\text{m}^3 \text{m}^{-3}$

Thickness of proposed barrier: 0.5(0.1) m

Hydrodynamic dispersivity: $8.75\text{E-}5(1.0\text{E-}4)$ m

Log van Genuchten's n: 0.11(0.02) $\log_{10}(\cdot)$

Temperature of soil (for computing molecular diffusivity): 11.7(7.38) Celsius

Soil bulk density: 1290000.0(168000.0) g m^{-3}

Mean soil particle radius: $9.95\text{E-}5(6.15\text{E-}5)$ m

Log Saturated hydraulic conductivity: $-2.09(0.48)$ $\log_{10}(\text{m h}^{-1})$

⁷ This was calculated as ca. $0.9091 x_s$, where the value 0.9091 is the water saturation fraction at the field capacity for centroid clay texture (64.83% Clay, 16.55% Silt, 18.62% Sand) calculated using the method on the website, <http://www.bsyses.wsu.edu/saxton/soilwater/>

Virus Parameters:

- Coefficient of exponential decay of input concentration: 0.1(1.0E-11) h⁻¹
- Log Mobile Virus Inactivation Rate: 0.605(0.608) log₁₀(h⁻¹)
- Log Solid-sorbed Virus Inactivation Rate: 0.304(0.608) log₁₀(h⁻¹)
- Mobile to solid-sorbed mass transfer coeff : 0.00134(0.0018) m h⁻¹
- Mobile to air-sorbed mass transfer coeff.: 0.00927(0.0018) m h⁻¹
- Radius of virus: 1.375E-8(1.25E-9) m
- Maximum virus concentration entering proposed barrier. 10.0(0.01) any
- Mobile to solid-sorbed equilibrium partition coeff.: 7.2E-4(9.74E-4) m³ g⁻¹
- Saturated water content: 0.515332222 (0.085260028) m³ m⁻³
- Thickness of proposed barrier: 0.5 (1.0E-4) m
- Hydrodynamic dispersivity: 8.75E-5 (1.0E-4) m
- Log van Genuchten's n: 0.113751456 (0.015201357) log₁₀(.)
- Temperature: 11.7 (7.38) °C
- Soil bulk density: 1290000.0 (168000.0) g m⁻³
- Mean soil particle radius: 9.95E-5 (6.15E-5) m
- Log Saturated hydraulic conductivity: -2.085670553 (0.475140674) log₁₀(m h⁻¹)

The probability of failure to achieve 4.0-log attenuation from 1000000 Monte Carlo runs was 60:1000000.

Again, the last entry gives the probability of failure to achieve successful reduction of virus concentration. Here the choice of a water content constantly equal to the field capacity yields a substantially higher probability of failure to attenuate.

Further Results

Runs for the thirteen possible default data sets are summarized in the table below. For clay and sand textures, 1000000 iterations were sufficient to estimate the probability of failure. For the silt texture, even the accumulated results from four simulations did not detect any failure cases.

Other mixed cases are shown in the table. These were computed using the textural based, flow parameters with a set of virus parameters. For example, the clay loam flow parameters were used with the polio-clay virus parameters

Table 3.1 Failures to Achieve 4-log₁₀ Attenuation Results for Various Soil Textures for a Single *Virulo* Simulation Run of 10⁶ Iterations

Texture	Poliovirus	Hepatitis A	Reovirus 3	Coxsackievirus	Echovirus
Clay, θ _m = UD	0	11	13	15	18
Clay, θ _m = FC = 0.468	60	31009	68383	79880	54778
Clay loam, θ _m = UD	0	6	7	10	10
Loam	1	3	9	7	8
Loamy sand	35	158	265	332	219
Sand, θ _m = UD	236	864	684	655	612
Sand, θ _m = FC = 0.133	0	1	0	0	0
Sand, θ _m = 0.35	98,358	277,415	232,229	228,397	220,645

UD = Uniform Distribution between θ_r and θ_s
 FC = Field Capacity Moisture Content

Section 4. References

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- U.S. EPA. 2000. National Primary Drinking Water Regulations. Ground Water Rule. *Fed. Regis.* 65(91) :30193-30274.

Section 5. Website References

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|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Centroid Compositions | http://www.epa.gov/superfund/programs/risk/airmodel/guide.pdf |
| Rosetta Database | http://www.ussl.ars.usda.gov/MODELS/Rosetta/rosetta.htm |
| Soil Texture Calculator | http://www.bsyse.wsu.edu/saxton/soilwater/ |
| Soil Texture Triangle | http://www.agronomy.psu.edu/Courses/SOILS101/Labs/texture.html |
| UNSODA and RETC | http://www.ussl.ars.usda.gov/ |

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