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VIRTUS, a Model of Virus Transport in Unsaturated Soils

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As a result of the recently proposed mandatory groundwater disinfection requirements to inactivate viruses in potable water supplies, there has been increasing interest in virus fate and transport in the subsurface. Several models have been developed to predict the fate of viruses in groundwater, but few include transport in the unsaturated zone and all require a constant virus inactivation rate. These are serious limitations in the models, as it has been well documented that considerable virus removal occurs in the unsaturated zone and that the inactivation rate of viruses is dependent on environmental conditions. The purpose of this research was to develop a predictive model of virus fate and transport in unsaturated soils that allows the virus inactivation rate to vary on the basis of changes in soil temperature. The model was developed on the basis of the law of mass conservation of a contaminant in porous media and couples the flows of water, viruses, and heat through the soil. Model predictions were compared with measured data of virus transport in laboratory column studies and, with the exception of one point, were within the 95% confidence limits of the measured concentrations. The model should be a useful tool for anyone wishing to estimate the number of viruses entering groundwater after traveling through the soil from a contamination source. In addition, model simulations were performed to identify parameters that have a large effect on the results. This information can be used to help design experiments so that important variables are measured accurately.

The significance of viruses as agents of groundwaterborne disease in the United States has been well documented (3, 4). The increasing interest in preventing groundwater contamination by viruses and other disease-causing microorganisms has led to new U.S. Environmental Protection Agency regulations regarding groundwater disinfection (21), the development of wellhead protection zones, and stricter standards for the microbiological quality of municipal sludge (20) and treated effluent (2) that are applied to land. For many of the new regulations, a predictive model of virus (or bacterial) transport would be helpful in the implementation process. For example, such a model could be used to determine where septic tanks should be placed or where land application of sludge or effluent should be practiced relative to drinking water wells to minimize negative impacts on the groundwater quality. Another application of microbial transport models is related to the groundwater disinfection rule (21). Water utilities wishing to avoid groundwater disinfection may use a pathogen transport model to demonstrate that adequate removal of viruses in the source water occurs during transport to the wellhead.

Several models of microbial transport have been developed during the past 15 to 20 years (6, 7, 11, 12, 17, 18, 23, 27). The models range from the very simple, requiring few input parameters, to the very complex, requiring numerous input parameters. For many of the more complex models (7, 11, 23), the data required for input are not available except for very limited environmental conditions. They may be useful for research purposes but would be impractical for widespread use. The potential applications of these models also range considerably, from being useful only for screening purposes on a regional scale (27) to predicting virus behavior at one specific location (6, 13, 18). One limitation of almost all of these models is that they have been developed to describe virus transport in saturated soils (i.e., groundwater). However, it has been demonstrated many times that the potential for virus removal is greater in the unsaturated zone than in the groundwater (9, 10, 14). If the viruses are transported through the unsaturated zone before entering the groundwater, then neglecting the unsaturated zone and assuming that the viruses immediately enter the saturated zone in a model of virus transport could lead to inaccurately high predictions of virus concentrations at the site of interest. This omission would be especially significant in areas with thick unsaturated zones, such as those in many western states. The one transport model (18) that has reportedly been developed for predicting virus transport in variably saturated media is not specific for viruses but can be used for any contaminant. In addition, it has not been tested with data of virus transport in unsaturated soil.

Another, more important limitation of published models of virus transport is that none of them has been validated by using actual data of virus transport in unsaturated soils. Most models are developed on the basis of theory and are fitted to data obtained from one or two experiments. Rarely are they tested by applying the model to data collected under a variety of conditions and by then determining how well the model predicts what has been observed in the laboratory or field without any fitting or calibration of the model.

The purpose of this research was to develop a model that can be used to predict virus movement from a contamination source through unsaturated soil to the groundwater. The model was tested by comparing the model predictions with the results of laboratory studies. Several model simulations were then performed to determine the effects of different input parameters on model predictions.

MATERIALS AND METHODS

Model development. The computer model, VIRTUS (virus transport in unsaturated soils), is a one-dimensional numerical finite difference code written in FORTRAN programming language. It simultaneously solves equations describ-

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ing the flow of water, viruses, and heat through unsaturated soil under different climatic conditions. The equation used to calculate the transport of water through the soil is

$$\frac{\partial}{\partial t}[\rho_w\theta + \rho_{wv}^{sat}(T)h(\varepsilon - \theta)] = -\nabla \cdot [\rho_w\theta V_l + \rho_{wv}(\varepsilon - \theta)V_v] \quad (1)$$

where t is time (in hours), ρ_w is the density of water (in grams per cubic centimeter), θ is the volumetric soil water content (in cubic centimeters per cubic centimeter), $\rho_{wv}^{sat}(T)$ is the density of water vapor at saturation at T (in grams per cubic centimeter), T is temperature (°C), h is the relative humidity at the atmosphere-soil interface (dimensionless), ε is the soil porosity (in cubic centimeters of soil voids per cubic centimeter of soil), V_l is the velocity of water in the liquid phase (in centimeters per hour), and V_v is the velocity of water in the vapor phase (in centimeters per hour). Heat transport through the soil is calculated by using the equation

$$\frac{\partial}{\partial t}[(1 - \varepsilon)C_{solid}\rho_{solid}T + (\varepsilon - \theta)c_{air}\rho_{air}T + \theta C_w\rho_w T] = -\nabla \cdot [(1 - \varepsilon)H_{ss} + \theta H_{sl} + (\varepsilon - \theta)H_{sv}] \quad (2)$$

where c_{solid} is the specific heat of the solid (in calories per gram per degree Celsius) (1 cal = 4.184J), ρ_{solid} is the density of the solid (in grams per cubic centimeter), c_{air} is the specific heat of the air (in calories per gram per degree Celsius), ρ_{air} is the density of the air (in grams per cubic centimeter), c_w is the specific heat of the water (in calories per gram per degree Celsius), H_{ss} is the transfer of heat by conduction through the soil particles (in calories per square centimeter per hour), H_{sl} is the transfer of heat by conduction and convection in the liquid-phase water (in calories per square centimeter per hour), and H_{sv} is the transfer of heat by conduction in the vapor-phase water and by transport in the form of latent heat (in calories per square centimeter per hour). The equation governing the transport of viruses through the soil is given by:

$$\frac{\partial}{\partial t}(\rho_b C_s + \theta C_l) = \frac{\partial}{\partial z}\left(\theta D\frac{\partial C_l}{\partial z}\right) - V_l\theta\frac{\partial C_l}{\partial z} - (\theta\mu_l C_l + \rho_b\mu_s C_s) - \theta f C_l \quad (3)$$

where ρ_b is the bulk density of the soil (in grams per cubic centimeter), C_s is the concentration of viruses adsorbed to the soil (in PFUs per gram of solid), C_l is the concentration of viruses suspended in the liquid phase (in PFUs per milliliter), D is the hydrodynamic dispersion coefficient (in square centimeters per hour), μ_l is the inactivation rate of viruses in the liquid phase (per hour), μ_s is the inactivation rate of adsorbed viruses (per hour), f is the filtration coefficient (per centimeter), and z is the position in space (in centimeters). The derivations of these equations are given by Ouyang (13) and Yates et al. (29).

The processes used in the model to describe virus fate and transport include advection (transport by the bulk movement of water), dispersion (spreading out of the viruses as they move around soil particles), adsorption, inactivation, and filtration. A complete discussion of these factors and their effects on microbial transport has been published recently (28). Some of the specific features of the model will now be described.

In the model, advection and dispersion of the virus particles are allowed to vary as the viruses are transported through the soil profile. In other words, the rate at which viruses are transported through the soil varies on the basis of the velocity of the water, which depends on the flow of heat through the system, among other factors. Another attribute of VIRTUS is that the user may input different virus inactivation rates for viruses that are adsorbed to the soil particles as compared with freely suspended viruses, if that information is known.

One important feature of the model is that the inactivation rate does not have to remain constant throughout the simulation. Because the model simulates the flow of heat through the soil, it allows one to compute a new value for any heat-dependent variable as the temperature changes in the soil profile. It has been well documented that virus inactivation rates are temperature dependent (8, 16, 24). An equation describing the relationship between virus inactivation rates and subsurface temperatures has been developed previously (25) and is

$$\mu = -0.181 + (0.0214 \times T) \quad (4)$$

where μ is the inactivation rate of the viruses (in $\log_{10}$ per day) and T is the temperature (°C). Thus, whenever the temperature of the soil changes, VIRTUS calculates a new virus inactivation rate on the basis of this equation. The user may specify the virus inactivation rate to be a constant or a function of any of the variables in the program. Equation 4 was used in several of the examples that will be presented herein.

Model testing. The model was tested for its ability to predict virus movement measured in laboratory column studies. Three data sets that contained sufficient information about the soil properties for the model were obtained. In examples 1 and 2, the data were obtained from virus transport experiments using saturated soil columns conducted by Grondin at the University of Arizona, Tucson (5). For example 3, the data were obtained from virus transport experiments using unsaturated soil columns conducted by Powelson at the University of Arizona, Tucson, and reported by Powelson et al. (14). The data used as model input for each example are listed in Table 1.

In each case, the model was run by using input values measured or reported by the respective investigator. Model predictions were then compared with the virus concentrations measured as a function of soil depth and time in the laboratory.

Model simulations. Several features of the model were demonstrated by using data for two different soil types, a loam (example 4) and a sand (example 5). Some of the input data for these examples are shown in Table 2. Soil data were obtained from Ouyang (13) for the Indio loam and from Ungs et al. (19) for the Rehovot sand. Virus data were obtained from several sources (1, 6, 14, 26) reporting virus transport characteristics in soils similar to those used in the model. In all simulations, water was added to the soil columns at a rate of 0.1 cm h^{-1} for 6 h. The concentration of viruses in the influent solution was 10^5 PFU ml^{-1}.

In example 4, the effects of three different virus inactivation rates on model predictions were determined. For example 4a, the virus inactivation rate varied as a function of the soil temperature throughout the simulation. Virus inactivation rates were calculated by using equation 4. For examples 4b and 4c, the virus inactivation rates were calculated for constant soil temperatures of 10 and 25°C, respectively. In these three examples, virus inactivation was calculated only

TABLE 1. Data used for model testing[a]

Property	Input value		
	Example 1	Example 2	Example 3
Soil type	Gravelly sand	Gravelly sand	Loamy fine sand
Soil bulk density (g cm $^{-3}$)	1.65 g	1.65	1.54
Hydrodynamic dispersion (cm^2 h $^{-1}$)	78	59	92.24
Soil water content (cm^3 cm $^{-3}$)	0.26	0.26	Variable with depth
Average water velocity (cm h $^{-1}$)	48.3	28.3	1.54
Soil column length (cm)	100	100	100
Soil adsorption coefficient ($K_d = C_s/C_l$) (ml g of soil $^{-1}$)	−0.054	−0.073	0.27
Virus type	MS2 coliphage	MS2 coliphage	MS2 coliphage
Virus inactivation rate ($\log_{10}$ day $^{-1}$)	0.082	0.056	2.00
Filtration coefficient (cm $^{-1}$)	0	0	0
Input virus concentration (PFU ml $^{-1}$)	6.3×10^3	8.37×10^3	10^5
Simulation time	48 min	48 min	4 days

[a] From Grondin (5) and Powelson et al. (14).

for the freely suspended viruses, while the inactivation rate of viruses adsorbed to soil particles, μ_s, was zero. In example 4d, the inactivation rate of adsorbed viruses was specified to be one-half of the rate for viruses suspended in the water, μ_l, which changed as a function of soil temperature (i.e., same as example 4a with a μ_s of $0.5\mu_l$).

Example 5 simulates the transport of viruses through a sandy soil. In this example, the virus inactivation rate for freely suspended viruses changed as a function of temperature as described in equation 4 with a μ_s of 0.

RESULTS

Examples 1 and 2. Figure 1 shows the predicted virus concentrations at several depths after 48 min of transport in a saturated column of gravelly sand. The model predictions were close to the measured virus concentrations and in all cases fell within the 95% confidence limits of the measured data. In the second example, the model predictions were within the 95% confidence limits of the measured data at all points except the 100-cm depth (Fig. 2). Compared to the measured virus concentrations, the model overpredicted the concentration of viruses that would be present in the column outflow. Grondin (5) measured 0 PFU of viruses after 48 min, while the model predicted, on the basis of Grondin's data, that the virus concentration would be 341 PFU ml $^{-1}$.

Example 3. Virus transport in an unsaturated soil column of loamy fine sand, with measured values provided by Powelson et al. (14), is depicted in Fig. 3. The agreement between model predictions and the observed data is very good in this case. The model predicted that the virus concentration in the column outflow after 4 days would be 3.54 $\log_{10}$ PFU ml $^{-1}$, while the measured concentration was 3.78 $\log_{10}$ PFU ml $^{-1}$.

TABLE 2. Data used for model simulations

Property	Input value[a]	
	Example 4	Example 5
Soil type	Indio loam	Rehovot sand
Soil bulk density (g cm^{-3})	1.2	1.595
Hydrodynamic dispersion	f(velocity)	f(velocity)
Initial soil water content (cm^3 cm^{-3})	0.25	0.1
Residual soil water content (cm^3 cm^{-3})	0.029	0.008
Initial soil temp (°C)	8.7	8.7
Saturated hydraulic conductivity (cm h^{-1})	0.61	52.89
Soil column length (cm)	100	100
Soil adsorption coefficient ($K_d = C_s/C_l$) (ml g of soil^{-1})	0.27	0
Virus type	MS2 coliphage	MS2 coliphage
Virus inactivation rate (free) (μ_l)		
Example 4a	f(temperature)	f(temperature)
Example 4b	0.033 $\log_{10}$ day^{-1}	
Example 4c	0.354 $\log_{10}$ day^{-1}	
Example 4d	f(temperature)	
Virus inactivation rate (adsorbed) (μ_s)		
Example 4a	0	0
Example 4b	0	
Example 4c	0	
Example 4d	$0.5 \times \mu_l$	
Input virus concentration (PFU ml^{-1})	10^5	10^5
Filtration coefficient (cm^{-1})	0	0

[a] Values were obtained from references 1, 6, 13, 14, 19, and 26.

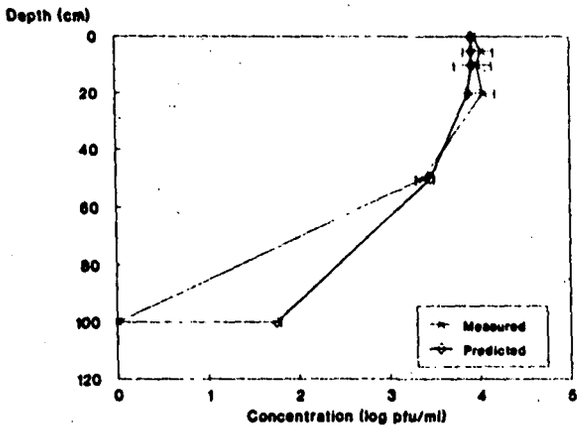

FIG. 1. Comparison of model predictions with experimental data of Grondin (5) for a saturated, gravelly sand soil (example 1). Ninety-five percent confidence limits were calculated from seven replicates.

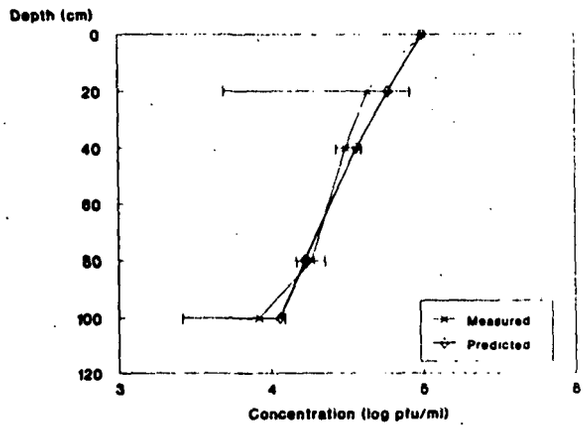

FIG. 3. Comparison of model predictions with experimental data of Powelson et al. (14) for a loamy fine sand soil (example 3). Ninety-five percent confidence limits were calculated from seven replicates.

Example 4. Virus concentrations in the 100-cm-long column of loam soil predicted by using a variable inactivation rate are shown in Fig. 4. Four different curves are shown, representing snapshots of the virus concentration profile in the column after 6, 24, 72, and 120 h of transport. Figures 5a and b show the effects of the different inactivation rates on model predictions of virus transport. In Fig. 5a, the difference in the concentration of virus particles predicted by using a variable inactivation rate and the constant rate at 10°C is shown. The difference between predicted concentrations by using the variable, temperature-dependent inactivation rate and the constant rate at 25°C is shown in Fig. 5b.

The differences in virus concentrations predicted by the model when the rate of inactivation of adsorbed viruses is zero compared to when the rate of inactivation of adsorbed viruses is assumed to be one-half that of the free viruses are shown in Fig. 6.

Example 5. Model predictions of virus transport in a soil column of Rehovot sand with the virus inactivation rate calculated as a function of temperature as described in equation 4 are shown in Fig. 7.

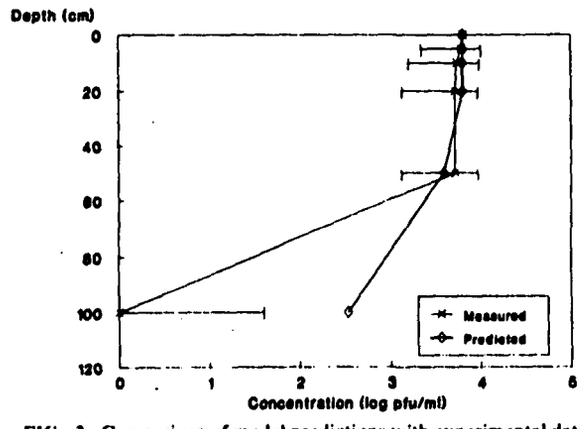

FIG. 2. Comparison of model predictions with experimental data of Grondin (5) for a saturated, gravelly sand soil (example 2). Ninety-five percent confidence limits were calculated from seven replicates.

DISCUSSION

Model testing. The ultimate measure of the usefulness of a model as a predictive tool is its ability to accurately predict field observations of virus transport under a variety of environmental conditions. However, most models that have been developed to predict microbial transport have not been tested by using field or laboratory data. There are a few exceptions to this. For example, Teutsch et al. (17) developed a one-dimensional model to describe microbial transport that includes decay, growth, filtration, and adsorption. The model predictions compared closely with the measured

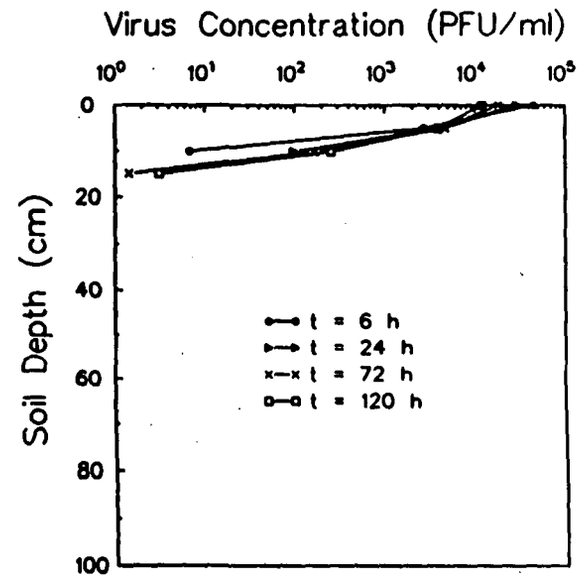

FIG. 4. Virus concentration as a function of soil depth when a temperature-dependent inactivation rate was used with an Indio loam soil (example 4a).

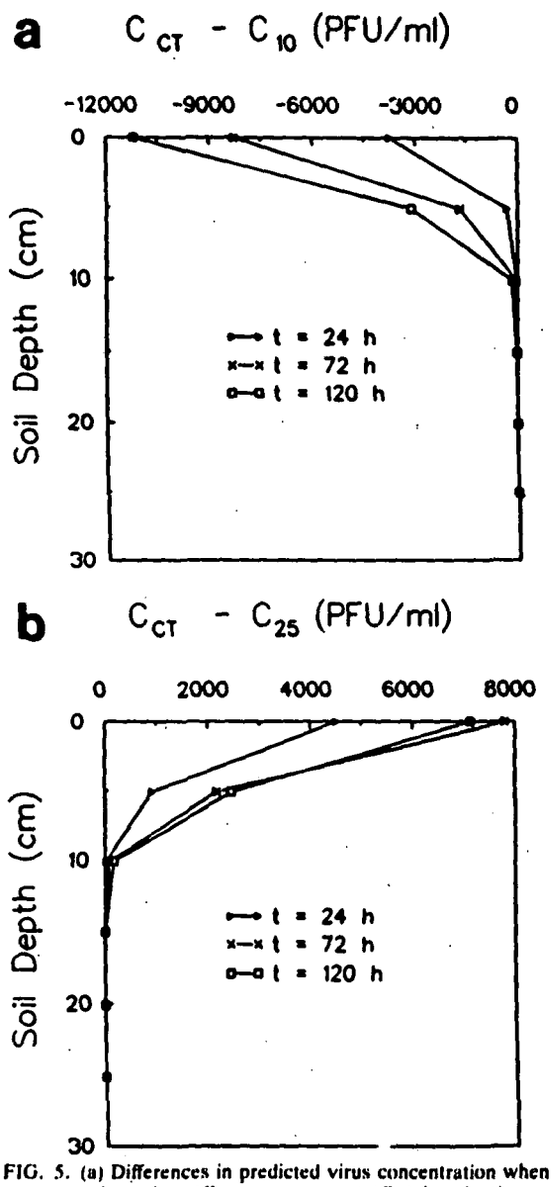

FIG. 5. (a) Differences in predicted virus concentration when a temperature-dependent (C_{ct}) or a constant (C_{10}) inactivation rate was used with an Indio loam soil (example 4a versus 4b). (b) Differences in predicted virus concentration when a temperature-dependent (C_{ct}) or constant (C_{25}) inactivation rate was used with an Indio loam soil (example 4a versus 4c).

results of a high-flow-rate experiment of MS2 transport. However, at low flow rates, microbial behavior could not be simulated closely by using the same transport equation. Harvey and Garabedian (7) simulated bacterial transport by using a colloid filtration model that had been modified to include advection, storage, dispersion, and adsorption. They compared model predictions with measurements of bacterial transport in a sandy aquifer in Cape Cod, Mass. While the model was able to simulate the bacterial transport measured at a sampling point at a depth of 9.1 m, model predictions for a sampling point at a depth of 8.5 m were not very close to the measured concentrations, especially at later times.

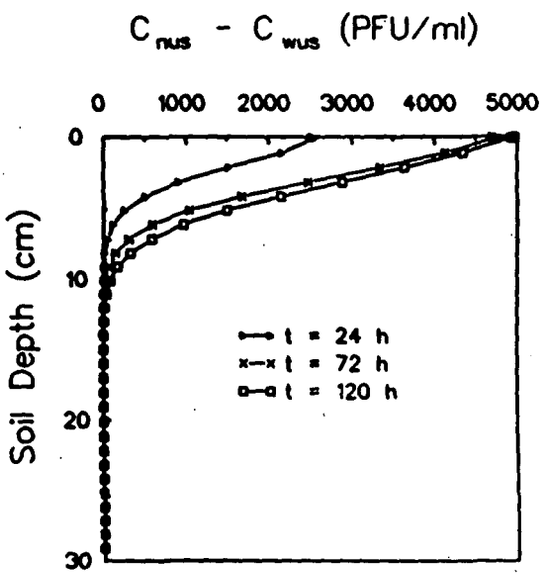

FIG. 6. Effects of assuming no inactivation of adsorbed viruses (C_{nus}) or of assuming a nonzero inactivation rate of adsorbed viruses (C_{wus}) on model predictions for an Indio loam soil (example 4a versus 4d).

Both of these models were developed for use by the investigators to simulate their own data. In the case of the colloid filtration model, extensive fitting of the required input parameters was performed by calibrating different solutions of the transport equation to the observed bacterial breakthrough curves (7). Thus, while these models may be able to simulate the data of the investigator reasonably well, they may not be able to predict the results of the transport

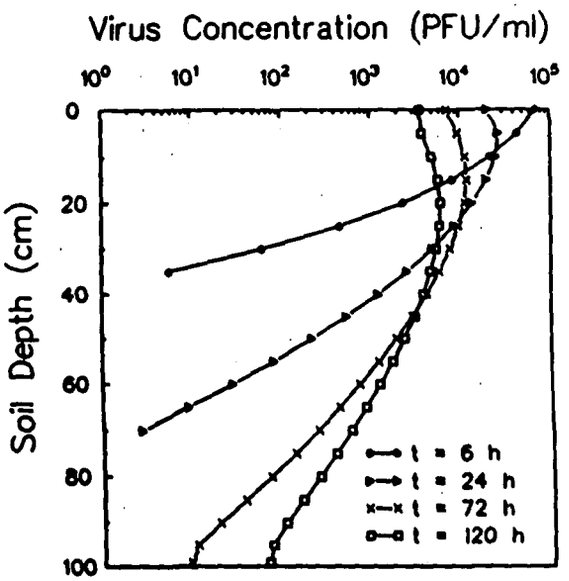

FIG. 7. Virus concentration as a function of soil depth when a temperature-dependent inactivation rate was used with a Rehovot sand soil (example 5).

experiments of other investigators. If a model is to be used for purposes other than research, such as community planning or making regulatory decisions, it must be able to predict microbial transport by using data obtained by anyone under a wide range of environmental conditions.

Tim and Mostaghimi (18) attempted to simulate the results of a saturated-flow column transport experiment using poliovirus 1 conducted by Lance and Gerba (10). They used a conventional equation for describing solute transport, i.e., the advection-dispersion equation, in their studies. The difficulty encountered by these investigators was that insufficient data were reported by Lance and Gerba (10) to fulfill the input requirements of the model. Therefore, they had to estimate values for the virus adsorption coefficient, the virus inactivation rate, the saturated hydraulic conductivity, the hydrodynamic dispersion coefficient, the moisture content at saturation, and the average porosity of the soil. The model simulation of virus concentrations compared closely to the measured virus concentrations in the top 80 cm of the soil column; however, because so many of the input values were estimated, it is difficult to assess the accuracy of the model.

In this research, a model to describe virus transport was developed on the basis of the factors known to affect virus fate in the subsurface. A survey of the literature was conducted to locate data sets in which the investigators made measurements of not only virus properties but also soil and hydraulic properties. Three data sets were located and used to test VIRTUS. No fitting or calibration of the model was performed; the data and measurements as reported by the respective investigators were used as model input.

When the predictions of VIRTUS were compared with the results obtained by Grondin (5) by using a saturated gravelly sand column, the model predictions were within the 95% confidence limits of the measured virus concentrations for one trial (Fig. 1). For the second trial, the model predicted that more than 300 viruses ml^{-1} would appear in the column effluent after 48 min, although none were detected in the laboratory study (Fig. 2). The discrepancy between the model predictions and the laboratory measurements may be due to the reported value for the adsorption coefficient (-0.54 ml g of $soil^{-1}$). This value was not measured by the investigators by using a batch adsorption isotherm study; rather, the value was used as a fitting parameter for their data. In the model, a negative value for the adsorption coefficient would have the effect of transporting the viruses at a more rapid rate through the soil (on average) than the average velocity of the water and resulted in viruses being present in the column effluent. If, in reality, there was adsorption of the viruses to the soil particles, this would retard their movement through the column and result in no viruses being detected in the outflow.

In the case in which VIRTUS was tested by using the data of Powelson et al. (14), model predictions were very close to the measured virus concentration profiles (Fig. 3). However, this is only one example of a comparison to one laboratory transport study in unsaturated soil by using a single soil type and a single virus type. More testing of the model is required before it should be used for any purposes other than research.

Unfortunately, in these examples, the temperature-dependent inactivation rate capabilities of the model could not be tested. This is due to the fact that the experiments were conducted under constant temperature conditions in the laboratory, and, thus, the virus inactivation rate remained constant (theoretically) throughout the course of the experiment. To test the capacity of the model to calculate new virus inactivation rates as a function of the changing soil temperature, data from a laboratory study in which the temperature is allowed to change (and is closely monitored) or from a field study in which the temperature is monitored will be required. This will allow an assessment of the capability of the model to accurately calculate heat flow through the soil, which affects water flow (and thus virus transport) as well as the rate of virus inactivation during transport.

Model simulations. In addition to being predictive tools, models are useful for demonstrating the effects of different variables on model results. Because it is not feasible to perform experiments on all possible combinations of viruses, soil types, and environmental conditions to determine their transport behavior, models can serve as a useful alternative. The value of input variables can be easily changed, and the results on model outputs can be determined. For example, the model can be run by using different values for temperature while holding constant all other values. By using this technique, a quantitative measure of the influence of temperature on model results can be obtained. If it is shown that a given variable has a considerable effect on the model predictions, this indicates that experiments should be designed in such a way that the variable is measured accurately. Several factors that affect the transport and fate of viruses in the unsaturated zone, and which thus affect model predictions, were investigated by using model simulations and are discussed below.

(i) **Effects of temperature-dependent inactivation rates.** Most models of contaminant transport consider the movement of water and the transport of the contaminant in their development and assume that the thermal conditions in the soil remain constant. In reality, under field conditions, this is not generally the case. Temperature fluctuations in soil can be considerable throughout the course of a 24-h period, especially near the soil surface. Because the effects of temperature on virus inactivation rates in the environment can be quite significant, it seems logical to use a model of contaminant transport that also models heat flow.

The effects of allowing the virus inactivation rate to vary as a function of soil temperature in comparison with the effects of holding it constant are graphically shown in Fig. 5a and b. In the case where the virus inactivation rate was held constant at 0.033 $\log_{10}$ day^{-1} (10°C), the model predicted higher concentrations of viruses than would be predicted if the inactivation rate was allowed to vary as a function of temperature (Fig. 5a). The opposite predictions were obtained in the case of a constant inactivation rate of 0.354 $\log_{10}$ day^{-1} (25°C), as shown in Fig. 5b. When the inactivation rate was considered to be a constant at 25°C an underprediction in the concentration of viruses resulted as compared with that predicted when the inactivation rate was considered to be temperature dependent.

The reasons for these predictions become apparent upon observation of the predicted change in soil temperature that occurs as applied water is infiltrated through the soil column. Figure 8 shows the soil temperature as a function of time for the model simulations discussed for example 4 above. At the soil surface, over a 24-h period, the soil temperature (which started at 8.7°C) decreased to 3°C at 6 h during the addition of cold water and increased to 35°C at 12 h because of the effects of solar radiation. Similar patterns would be expected at the 5- and 10-cm depths, although the magnitude of the variation would not be as large. In example 4b, the virus inactivation rate was held constant at a value that would be expected for constant 10°C soil conditions. The fact that the

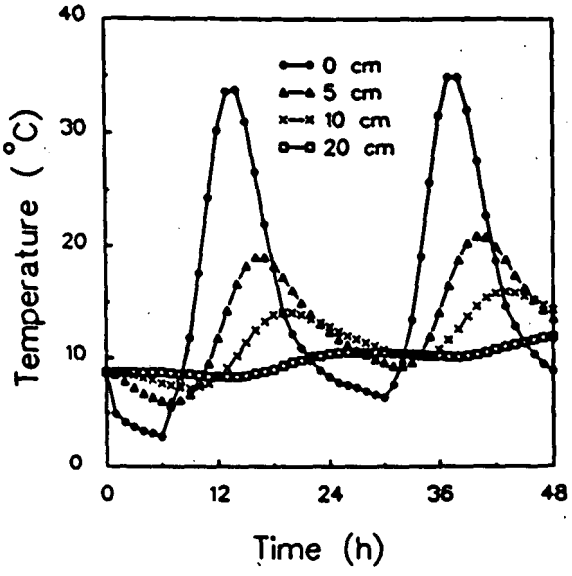

FIG. 8. Soil temperature as a function of time for an Indio loam soil (example 4).

soil temperature rose above 10°C for more than 12 h in a 24-h period resulted in a prediction of virus inactivation at relatively high rates (compared to the rate at a constant temperature of 10°C) for that period. Overall, maintaining the inactivation rate at a constant value had the effect of increasing the predicted concentration of viruses that were transported in the soil column by more than 4 orders of magnitude (Fig. 5a).

In example 4c, the soil temperature was considered to be constant at 25°C; consequently, the virus inactivation was maintained at a relatively high rate throughout the transport process. In actuality, the soil temperature was at or above 25°C for a relatively short period of time (less than 6 h), so viruses were inactivated at or above that high rate for only 6 h in the simulation where the rate was temperature dependent. In this case (Fig. 5b), an assumption of a constant inactivation rate would lead to a prediction that thousands of viruses fewer than the actual number (assuming that the variable inactivation rate simulation predicts the actual number) would be transported in the column.

The sensitivity of model predictions to changes in the temperature-dependent inactivation rate was determined by changing the inactivation rate while keeping all other variables constant. This sensitivity analysis showed that changing the value of the inactivation rate by 50% resulted in a 33% change in the predicted concentration of viruses being transported through the soil. A high sensitivity of model predictions to the virus inactivation rate has also been observed by Tim and Mostaghimi (18) and Park et al. (12). These results demonstrate the need to accurately monitor virus inactivation and/or temperature during experiments of virus transport in the subsurface.

(ii) Effects of inactivation rates for adsorbed versus those of free viruses. There have been reports in the literature of differences in the measured rates of virus inactivation for viruses that are adsorbed to soil particles as compared with those for viruses that are freely suspended in the liquid medium (8, 15, 22). Therefore, this model was developed to allow the user to input different values for inactivation rates for viruses in these two states. When a value for the inactivation rate of adsorbed viruses is specified, the model calculates the number of viruses adsorbed at a given time on the basis of the adsorption coefficient specified by the user and determines accordingly the number of viruses inactivated.

It is difficult to obtain a quantitative value for the relative difference between inactivation rates for adsorbed viruses and those for freely suspended viruses. For the purposes of illustration, a simulation with a value for adsorbed viruses equal to one-half that of free viruses (temperature dependent) was compared with a simulation in which the inactivation rate for adsorbed viruses was zero. As one would expect, the concentration of viruses transported through the soil column is larger when the solid-phase inactivation rate is zero than when it is one-half the liquid-phase rate. The difference increases with time, as shown in Fig. 6. In a system in which the inactivation rate of adsorbed viruses is equal to that of free viruses, the differences would be even greater.

This example demonstrates the importance of knowing the inactivation rate for viruses in the adsorbed and liquid phases. If the inactivation rate for adsorbed viruses is actually lower than that of suspended viruses, it would be important to incorporate that information in a model so that accurate predictions could be made of virus concentration profiles. If the model assumes the same inactivation rate for all viruses, it would predict that fewer viruses are being transported than the actual number.

(iii) Effects of soil type. A simulation of virus transport by using data for a Rehovot sand was run to illustrate the effects of soil properties on transport. The Rehovot sand has a much higher hydraulic conductivity (Table 2) than that of the Indio loam, and, thus, water and contaminants can move through this soil more rapidly. As shown in Fig. 7, the viruses were transported more rapidly and in higher concentrations in this soil than in the loam soil of the previous examples. After 6 h, the viruses in the loam soil had been transported only 11 cm (Fig. 4), in comparison to more than 35 cm in the sandy soil (Fig. 7). The differences between the two columns become more apparent at longer times: after 5 days, approximately 30 viruses ml^{-1} had been transported 15 cm in the loam soil, whereas more than 10^2 viruses ml^{-1} were being recovered in the sand column effluent after the same length of time.

Another reason for the relatively higher concentrations of viruses being transported through this soil, in addition to the higher hydraulic conductivity, is related to the adsorption coefficient. For this sand, on the basis of reported values for virus adsorption to other sandy soils, an adsorption coefficient of zero was chosen. Thus, the rate at which the viruses were transported through the soil was not decreased as a result of adsorption to the soil particles, unlike the case for the loam soil.

Conclusions. A model of virus transport, VIRTUS, that simultaneously solves equations describing the transport of water, heat, and viruses through the unsaturated zone of the soil has been developed. The effects of a temperature-dependent inactivation rate versus a constant inactivation rate were shown to be considerable in terms of the concentrations of viruses that are predicted to be transported. In addition, it was shown that different inactivation rates for adsorbed versus freely suspended viruses may have a considerable effect on model predictions. More data on the relative inactivation rates for viruses in these two states are necessary so that model input values are as accurate as possible.

VIRTUS was tested by using three data sets obtained during laboratory studies of coliphage transport and was found to produce reasonable predictions in comparison with measured results. However, before this or any model of contaminant transport can be used with confidence for any purpose other than research, considerable testing is required. VIRTUS must be tested by using field data collected in a wide variety of environmental and hydrogeologic settings, so that its limitations can be assessed. Few, if any, data sets containing both virus data and the appropriate hydrogeologic data are currently available so that this, or any, model can be tested. More transport studies using human viruses that have been implicated in waterborne disease outbreaks and bacteriophages must be conducted to assess the appropriateness of using phages or other microorganisms as surrogates for animal viruses in environmental fate studies.

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REFERENCES

1. **Bales, R. C., C. P. Gerba, G. H. Grondin, and S. L. Jensen.** 1989. Bacteriophage transport in sandy soil and fractured tuff. Appl. Environ. Microbiol. 55:2061–2067.
2. **California Department of Health Services.** 1990. Initial statement of reasons for proposed changes in the regulations of the Department of Health Services pertaining to the use of reclaimed water other than for groundwater recharge and pertaining to use of household gray water at residences and text of proposed regulations. California Department of Health Services, Sacramento.
3. **Craun, G. F.** 1986. Waterborne diseases in the United States. CRC Press, Boca Raton, Fla.
4. **Craun, G. F.** 1990. Review of the causes of waterborne disease outbreaks, p. 1–22. *In* G. F. Craun (ed.), Methods for the investigation and prevention of waterborne disease outbreaks. U.S. Environmental Protection Agency publication no. EPA/600/1-90/005a. U.S. Environmental Protection Agency, Washington, D.C.
5. **Grondin, G. H.** 1987. Transport of MS-2 and f2 bacteriophage through saturated Tanque Verde wash soil. M.S. thesis. University of Arizona, Tucson.
6. **Grosser, P. W.** 1984. A one-dimensional mathematical model of virus transport, p. 105–107. *In* Proceedings of the Second International Conference on Groundwater Quality Research, Tulsa, Okla.
7. **Harvey, R. W., and S. P. Garabedian.** 1991. Use of colloid filtration theory in modeling movement of bacteria through a contaminated sandy aquifer. Environ. Sci. Technol. 25:178–185.
8. **Hurst, C. J., C. P. Gerba, and I. Cech.** 1980. Effects of environmental variables and soil characteristics on virus survival in soil. Appl. Environ. Microbiol. 40:1067–1079.
9. **Keswick, B. H., and C. P. Gerba.** 1980. Viruses in groundwater. Environ. Sci. Technol. 14:1290–1297.
10. **Lance, J. C., and C. P. Gerba.** 1984. Virus movement in soil during saturated and unsaturated flow. Appl. Environ. Microbiol. 47:335–337.
11. **Matthess, G., A. Pekdeger, and J. Schroeter.** 1988. Persistence and transport of bacteria and viruses in groundwater—a conceptual evaluation. J. Contam. Hydrol. 2:171–188.
12. **Park, N., T. N. Blandford, M. Y. Corapcioglu, and P. S. Huyakorn.** 1990. VIRALT: a modular semi-analytical and numerical model for simulating viral transport in ground water. Office of Drinking Water, U.S. Environmental Protection Agency, Washington, D.C.
13. **Ouyang, Y.** 1990. Dynamic mathematical model of oxygen and carbon dioxide exchange between soil and atmosphere. Ph.D. dissertation. Oregon State University, Corvallis.
14. **Powelson, D. K., J. R. Simpson, and C. P. Gerba.** 1990. Virus transport and survival in saturated and unsaturated flow through soil columns. J. Environ. Qual. 19:396–401.
15. **Sobsey, M. D., C. H. Dean, M. E. Knuckles, and R. A. Wagner.** 1980. Interactions and survival of enteric viruses in soil materials. Appl. Environ. Microbiol. 40:92–101.
16. **Sobsey, M. D., P. A. Shields, F. H. Hauchman, R. L. Hazard, and L. W. Caton III.** 1986. Survival and transport of hepatitis A virus in soils, groundwater and wastewater. Water Sci. Technol. 18:97–106.
17. **Teutsch, G., K. Herbold-Paschke, D. Tougianidou, T. Hahn, and K. Botzenhart.** 1991. Transport of microorganisms in the underground—processes, experiments, and simulation models. Water Sci. Technol. 24:309–314.
18. **Tim, U. S., and S. Mostaghimi.** 1991. Model for predicting virus movement through soils. Ground Water 29:251–259.
19. **Ungs, M. J., L. Boersma, and S. Akratanakul.** 1985. OR-Nature: the numerical analysis of transport of water and solutes through soil and plants, vol. 4. Examples. Special report 754. Agricultural Experiment Station, Oregon State University, Corvallis.
20. **U.S. Environmental Protection Agency.** 1989. Standards for the disposal of sewage sludge; proposed rule. Fed. Regist. 54:5746–5902.
21. **U.S. Environmental Protection Agency.** 1991. Possible requirements of the ground-water disinfection rule. 20 June 1991. Office of Ground Water and Drinking Water, Washington, D.C.
22. **Vaughn, J. M., and E. F. Landry.** 1983. Viruses in soils and groundwater, p. 163–210. *In* G. Berg (ed.), Viral pollution of the environment. CRC Press, Boca Raton, Fla.
23. **Vilker, V. L., and W. D. Burge.** 1980. Adsorption mass transfer model for virus transport in soils. Water Res. 14:783–790.
24. **Yates, M. V., C. P. Gerba, and L. M. Kelley.** 1985. Virus persistence in groundwater. Appl. Environ. Microbiol. 49:778–781.
25. **Yates, M. V., and S. R. Yates.** 1987. A comparison of geostatistical methods for estimating virus inactivation rates in ground water. Water Res. 21:1119–1125.
26. **Yates, M. V., and S. R. Yates.** 1988. Modeling microbial fate in the subsurface environment. Crit. Rev. Environ. Control 17:307–344.
27. **Yates, M. V., and S. R. Yates.** 1989. Septic tank setback distances: a way to minimize virus contamination of drinking water. Ground Water 27:202–208.
28. **Yates, M. V., and S. R. Yates.** 1990. Modeling microbial transport in soil and groundwater. ASM News 56:324–327.
29. **Yates, M. V., S. R. Yates, and Y. Ouyang.** 1991. Development of a model of virus transport in unsaturated soils. Final report to R. S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, Okla.