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Behavior Assessment Model for Trace Organics in Soil: II. Chemical Classification and Parameter Sensitivity[1]

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ABSTRACT

this paper, the organic chemical transport screening model de- ·ed in Jury et al. (1983) is simplified by dividing chemicals into ilization and mobility categories. The volatilization classification ed on whether or not the predominant resistance to volatilization ies in the soil or in the boundary layer above the soil surface. This orization reduces to a condition on the Henry's constant (K_H) organic C partition coefficient (K_{oc}) when standard values are to represent soil and chemical parameters. The mobility cate- s are based on the calculated time to convect or diffuse a given nce through the soil.

mulations are conducted for chemicals falling into one or another iese volatilization or mobility categories to examine the sensitivity hese processes to variations in water evaporation, water content, inic C fraction, and boundary layer thickness. The dependence of volatilization flux and leaching flux on these parameters is sum- ized.

dditional Index Words: **chemical movement, diffusion, volatili- on, leaching.**

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a previous paper (Jury et al., 1983), we introduced a eening model for describing pesticide volatilization, ching, and degradation in soil. The soil surface undary consisted of a stagnant boundary layer con- cting the soil and air through which pesticide and iter vapor must move to reach the atmosphere. As- ming constant water flow and uniform soil properties, derived an analytical solution, which describes pesti- le concentration and flux as a function of chemical, vironmental, and soil properties.

In its present form, the theory is too complex to allow simple analysis to be made of the influence of soil and anagement properties on chemical behavior. Further- ore, it is not clear to what extent uncertainties in the lues of the measured chemical properties will influ- ice the predictions made by the model. Since our pro- osed use of the model will be as a screening tool to assify pesticides and other trace organics, such knowl- dge of input parameter sensitivity is essential. In this aper we examine the three major loss pathways: de- radation, mobility, and volatilization, and simplify the eneral theory in such a way as to allow general pesti- ide classification into specific behavioral groups. Vithin these groups, we will conduct a sensitivity nalysis that will examine the influence of various soil nd chemical properties on the loss pathways.

THEORY

Degradation

The processes contributing to biological or chemical gradation of an organic compound in soil are com- x, and their functional dependence on such soil and environmental parameters as water content, temperature, organic C, and soil pH are not well understood (Hamaker, 1972). In the absence of such quantitative information, the degradation potential of a given chemical is described with an effective first-order rate constant, μ, or half-life, $T_{1/2}$ (Nash, 1980; Rao & Davidson, 1980). This parameter represents the combined influence of degradation in all phases, and is usually measured by determining the fraction $M(T)/M(0)$ of a given initial quantity of applied chemical $M(0)$ remaining after a time t according to Eq. [1]

$$M(t) = M(\text{o}) \exp(-\mu t). \qquad [1]$$

Published measurements of μ differ widely (Hamaker, 1972; Nash, 1980; Rao & Davidson, 1980), not only because of different conditions, but because the degradation process may not best be described as first-order, or because unmeasured volatilization losses and soil measurement errors may interfere with the measurement of degradation losses by Eq. [1]. Nevertheless, the first-order rate coefficient is useful as a relative index of persistence.

In the model of Jury et al. (1983), the soil concentrations and surface volatilization fluxes are proportional to the factor exp $(-\mu t)$. The uncertainty in μ is likely to be as high as 100% or more (Nash, 1980), which could create a large error in the estimates made for compounds with short half-lives (large μ).

Mobility

CONVECTIVE MOBILITY

In the model of Jury et al. (1983), it was shown that a chemical with a linear, equilibrium partitioning between its vapor, liquid, and adsorbed phases will move with convective velocity

$$V_E = J_W/R_L = J_W/(\varrho_b K_D + \Theta + aK_H). \qquad [2]$$

The ratio of the total concentration to the liquid concentration is R_L, where J_W is water flux, K_D is adsorbed-liquid distribution coefficient, ϱ_b is soil bulk density, K_H is Henry's constant, a is volumetric air content, and Θ is volumetric water content. When the model is used to conduct leaching screening tests, the convective mobility may be classified in a variety of ways. One useful index, in analogy with chromatography, is to define a convection time t_c to move a distance l when a water flux J_W is present (Eq. [3]).

$$t_c = l/V_E = (\varrho_b K_D + \Theta + aK_H)\, l/J_W. \qquad [3]$$

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When adsorption is relatively high [i.e., $K_D > 4 \times 10^{-3}$ (m³/kg)], the water content Θ and aK_H may be neglected and t_c will be proportional to K_D and ϱ_b. For chemicals such as nonionic pesticides, which primarily adsorb to organic matter, the distribution coefficient K_D may be written as $f_{oc}K_{oc}$, where f_{oc} is organic C fraction and K_{oc} is organic C partition coefficient. In this case,

$$t_c \approx \varrho_b f_{oc} K_{oc} l / J_W. \qquad [4]$$

This convection time is a useful index of relative mobility and also will approximately describe the movement of a front or of the peak of a narrow pulse of chemical.

DIFFUSIVE MOBILITY

When mass flow by convection is small or negligible, the chemical is able to move through the soil only by liquid or vapor diffusion. In analogy with the convection time, we may define a characteristic diffusion time t_D to move a distance l, which may be written as (Carslaw & Jaeger, 1959).

$$t_D = l^2/D_E, \qquad [5]$$

where D_E is the effective soil diffusion coefficient (m²/d), given in Jury et al. (1983) as

$$D_E = \frac{D_G^{\text{air}} K_H a^{10/3}/\phi^2 + D_L^{\text{water}} \Theta^{10/3}/\phi^2}{\varrho_b K_D + \Theta + aK_H}, \qquad [6]$$

where K_H is Henry's constant, D_G^{air} is gaseous diffusion coefficient in air, D_L^{water} is liquid diffusion coefficient in water, a is air content, and ϕ is porosity. Only those chemicals that move predominantly in the vapor phase will have a relatively small t_D. For these chemicals, the first term in Eq. [6] dominates the second, and Eq. [5] may be written as

$$t_D \approx (\varrho_b f_{oc} K_{oc} + \Theta + aK_H)\,\phi^2 l^2 / D_G^{\text{air}} K_H a^{10/3}. \qquad [7]$$

Unlike the convection time t_c, this index will strongly depend on water or air content.

Volatilization

As described in our previous paper (Jury et al., 1983), the soil and atmosphere are connected by a stagnant air boundary layer through which water vapor and chemical vapor are assumed to move by diffusion. The extent to which this boundary layer limits the volatilization flux may be used as a criterion for classifying pesticides and other volatile organics into general categories, similar to the volatilization groups used to classify chemical losses from water bodies (Smith et al., 1980, 1981). To achieve this, it is convenient to distinguish between processes where no water flow (E) is occurring ($E = 0$) and processes where both volatilization and evaporation are occurring.

CASE 1. NO WATER EVAPORATION $E = 0$

When a chemical is initially uniformly incorporated in the soil at a total concentration C_0 (g/m³), the maximum volatilization flux rate J_{V_1} through the soil surface to the atmosphere that could occur is given by Jury et al. (1980)

$$J_{V_1} = C_0 (D_E/\pi t)^{1/2}, \qquad [8]$$

Category I

where D_E is given in Eq. [6] and where t is time (days). This flux rate is that which would occur with no boundary layer resistance in the air or equivalently when the surface concentration $C_T(0,t)$ is held at zero for all $t > 0$.

When a boundary layer of thickness d is present, the maximum flux J_{V_2} that can move through the boundary layer occurs when no soil resistance is present and the gas concentration C_G at the soil surface is held at its initial value $C_G(\text{o}) = C_o/R_G$

$$J_{V_2} = D_G^{\text{air}} C_o / R_G d, \qquad [9]$$

Category III

where $R_G = R_L/K_H = (\varrho_b K_D + \Theta + aK_H)/K_H$ is the ratio of the total chemical concentration to the concentration in the vapor phase. Equation [9] assumes that the concentration of the chemical in the free air above the boundary layer is zero.

When a boundary layer is present, it will act to restrict volatilization fluxes only if the maximum flux through the boundary layer J_{V_2} is small compared with the rate at which chemical moves to the soil surface, which we may represent approximately as J_{V_1}. Thus, if $J_{V_2} \ll J_{V_1}$, then

$$D_G^{\text{air}} C_o / R_G d \ll C_o (D_E/\pi t)^{1/2}. \qquad [10]$$

By plugging the definitions for R_G and D_E into Eq. [10], we may rewrite the condition expressed there in terms of the soil and chemical parameters in the various terms. To simplify the interpretation, we will use standard values for many of the soil and chemical properties other than the properties that differ greatly for different chemicals. These are summarized in Table 1.

When the soil water content is reasonably high (e.g., $\Theta > 0.2$), then the second term in the numerator of Eq. [6] will dominate the first term under the same circumstances (small K_H) when the inequality in Eq. [10] is valid. Thus, using $D_E \approx D_L/R_L$, we may rewrite Eq. [10] as

$$K_H^2/K_{oc} \ll \frac{D_L^{\text{water}} d^2 \Theta^{10/3}}{(D_G^{\text{air}})^2 \pi t \phi^2} \varrho_b f_{oc}, \qquad [11]$$

Table 1—Standard values of soil and chemical properties used in simulations.

Parameter	Symbol	Units	Standard value
Porosity	ϕ	m³/m³	0.5
Bulk density	ϱ_b	kg/m³	1350
Organic C fraction	f_{oc}	--	0.0125
Liquid diffusion coefficient	D_L^{water}	m²/d	4.3×10^{-5}
Air diffusion coefficient	D_G^{air}	m²/d	4.3×10^{-1}
Water content	Θ	m³/m³	0.3

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here it has been assumed in going from Eq. [10] to Eq. 1] that $R_L = \varrho_b K_D = \varrho_b f_{oc} K_{oc}$.

If we plug in the standard values from Table 1, along ith t = 2 d and d = 5 mm from Jury et al. (1983), we btain a benchmark criterion for a boundary layer inuence when volatilization occurs without water aporation

$$K_H^2/K_D \ll 9 \times 10^{-8}\,(\mathrm{kg/m^3}) \qquad [12]$$

ith $f_{oc} = 0.0125$.

ASE 2. WATER EVAPORATION $E \neq 0$

If upward water flow carries an insignificant amount f pesticide compared with upward diffusion, then the nalysis is identical to case 1. However, if upward conection is dominant, as it will be if the solution concenation is high, or if evaporation and volatilization both ccur for a long time period, then the upward flux of hemical J_{V_3} toward the boundary layer is approxiately equal to

$$J_{V_3} = C_L E \approx C_0 E/R_L, \qquad [13]$$

here C_L is solution concentration. The criterion for a oundary layer restriction on volatilization in this case ccurs when $J_{V_2} \ll J_{V_3}$, or

$$D_G^{\mathrm{air}} C_0/R_G d \ll C_0 E/R_L. \qquad [14]$$

rther, if we assume, as in Jury et al. (1983), that water aporation is also regulated by the boundary layer, we ay write a water vapor diffusion equation across the oundary layer as

$$E = [D_{wv}^{\mathrm{air}} \varrho_{wvs}(1 - \mathrm{RH})/2\varrho_{wL} d \qquad [15]$$

here ϱ_{wL} is liquid water density, ϱ_{wvs} is saturated water por density and RH is relative humidity. The factor of s inserted, as explained in Jury et al. (1983), because r model uses a steady-state evaporation flux, whereas rmal field evaporation rates are small during the ening hours. When Eq. [15] is plugged into Eq. [14] e obtain

$$ {}_H \ll [D_{wv}^{\mathrm{air}} \varrho_{wvs}(1 - \mathrm{RH})]/2D_G^{\mathrm{air}} \varrho_{wL} $$
$$ \approx 2.5 \times 10^{-5}. \qquad [16]$$

ote that Eq. [12] and [16] are identical for $K_D \approx 7 \times$ $0^{-3}\,(\mathrm{m^3/kg})$, which is a value representing moderate adrption.

Relationship to Chemical Volatilization from Water Bodies

Volatilization of dissolved chemicals from water dies has been modeled using a linear two-resistance m model (Liss & Slater, 1974), and by a two film del using penetration theory to represent transport m the liquid to the air water interface (Smith et al., 0, 1981). Irrespective of the model use, however, one ncludes that there is substantially less resistance to volatilization from the water body than has been found here (see Eq. [2]) for volatilization from soil. As a result, in water systems the air boundary layer forms a barrier to chemical loss at a much higher value of K_H than that predicted by Eq. [16] for soil systems. For example, the criterion equivalent to Eq. [16] obtained using the approach of Smith et al. (1981) for chemical loss from rivers is

$$K_H \ll 3.8 \times 10^{-3}. \qquad [17]$$

The reason that one obtains such a different answer in water bodies than in soil is that in a soil system upward chemical movement is restricted both by adsorption and by tortuosity effects (increased path length, decreased cross-sectional area) on diffusion compared with water transport. Since resistance to transport to the atmosphere through the stagnant air boundary layer is similar in both cases, the transition point where volatilization loss is regulated by the vapor phase shifts upward by over two orders of magnitude when water is analyzed instead of soil.

Pesticide Volatilization Categories

To simplify subsequent discussion, pesticides whose properties obey the inequalities Eq. [10] or Eq. [16] will be called category III, those whose properties obey the opposite inequality ($\gg$) will be called category I, and those for which Eq. [10] or Eq. [16] represent an equality will be called category II. Table 2 presents hypothetical but representative benchmark properties for pesticides in each of the three categories. For simplicity, each pesticide is given the same K_{oc}, water solubility (C_L^*), and μ, and Henry's constant K_H variations are achieved by varying saturated vapor density, C_G^*. With the above choices, the three pesticides fall unambiguously into different categories by both Eq. [10] and [16].

RESULTS

Mobility Classification

Equation [3] or [4] defines the dependence of the convective mobility time t_c on soil and chemical properties. To illustrate its use we may calculate the time required to move the chemical l = 10 cm when water is applied at J_W = 1.0 cm/d, for the standard conditions given in Table 1, with the result that $t_c \sim 170\,K_{oc} + 10\,\Theta$ (days). Thus, the chemicals 2,4-D [(2,4-dichlorophenoxy) acetic acid] and lindane (γ-1,2,3,4,5,6-hexachlorocyclo-

Table 2—Hypothetical pesticide benchmark properties and their categorical designation.

Property	Category I	Category II	Category III
Vapor density C_G^* (g/m^2)	10^{-1}	10^{-3}	10^{-5}
Solubility C_L^* (g/m^3)	40	40	40
K_{oc} (m^3/kg)	0.5	0.5	0.5
K_D (m^3/kg)	6.3×10^{-3}	6.3×10^{-3}	6.3×10^{-3}
μ (d^{-1})	0	0	0
K_H	2.5×10^{-3}	2.5×10^{-5}	2.5×10^{-7}
K^2_H/K_{oc}	1.25×10^{-5}	1.25×10^{-9}	1.25×10^{-13}

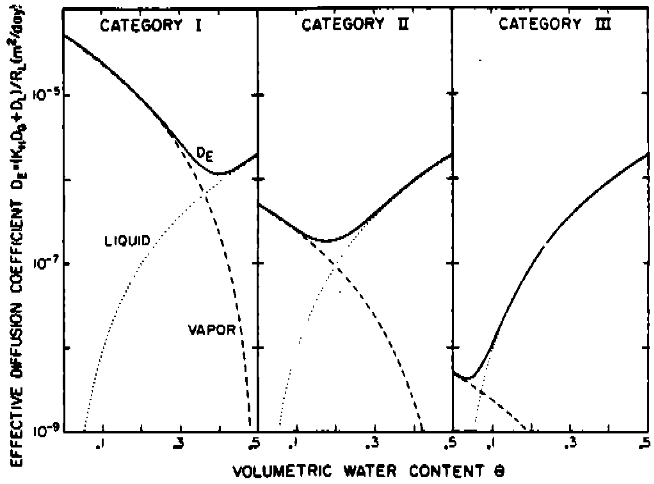

Fig. 1—Effective diffusion coefficients as a function of water content for prototype chemicals representing the three volatilization categories.

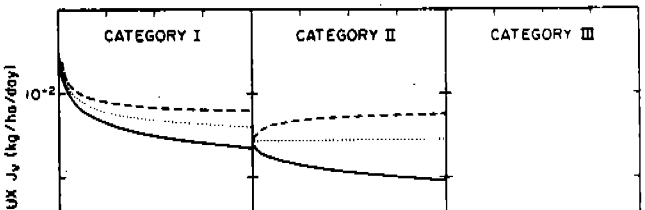

Fig. 2—Volatilization flux rates for the three chemical prototypes for three rates of water evaporation.

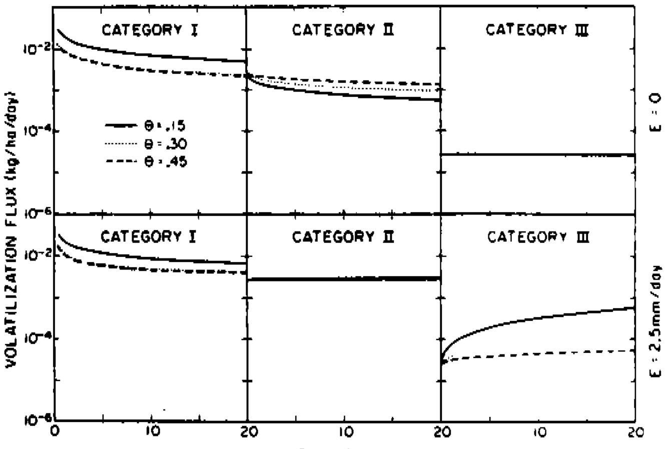

Fig. 3—Effect of changes in water content on volatilization flux rates for the three chemical prototypes. Top curves are for zero evaporation and bottom curves for evaporation of 2.5 mm/d.

hexane), which have $K_{oc} = 0.02$ and 1.3 m³/kg, respectively (Jury et al., 1983) have convective times of 6.4 and 224 d, respectively. These chemicals would represent highly mobile and relatively immobile compounds in a leaching classification scheme such as that of Helling (1971).

The diffusive mobility as defined by Eq. [7] will be important only for vapor dominated compounds with large K_H and small K_{oc}. To see this, if we require that in dry soil ($a \sim \phi$) the diffusive time to move 10 cm be < 20 d for a soil with properties given in Table 1; Eq. [7] reduces to the condition $K_{oc}/K_H < 20$. This condition is met only for fumigants and other vapor-dominated compounds of low adsorption. The compounds 2,4-D and lindane, for example, have $K_{oc}/K_H = 3.5 \times 10^6$ and 1×10^4, respectively (Jury et al., 1983).

Volatilization Classification

Figure 1 shows a plot of effective diffusion coefficient D_E (Eq. [6]) as a function of volumetric water content for the prototype chemicals (Table 2) chosen to represent the three categories. From this figure it is clear that a category I chemical is dominated by vapor diffusion and a category III chemical is dominated by liquid diffusion over most of the water content range. Category II chemicals are vapor-dominated at low water content and liquid-dominated at high water content.

Figure 2 shows volatilization flux rates vs. time for the three prototype chemicals under three cases of (i) no evaporation, (ii) steady evaporation at 2.5 mm/d, and (iii) steady evaporation at 5.0 mm/d. Again, a clear distinction is apparent between the behavior of category I and category III chemicals. For category I, the volatilization flux shows a characteristic decrease with time in all three cases, whereas the flux rate of the category III chemical tends to increase with time when upward water flow is occurring and to decrease slowly with time when evaporation is not present. The category II volatilization flux decreases with time when no evaporation occurs and increases with time when high evaporation occurs.

Figure 3 shows the influence of changes in water content on volatilization flux rates for the three chemicals for both volatilization without evaporation and volatilization with a water evaporation rate of 2.5 mm/d. The results suggest a very complicated dependence on water content for both cases. For example, category III chemicals show no water content dependence when water is not evaporating, but are strongly water content dependent when evaporation is occurring.

Figure 4 shows the effect of changing organic C fraction f_{oc} on volatilization flux rates. Since decreasing adsorption increases both convective and diffusive transport to the surface, in all cases volatilization increases with decreasing organic C fraction. However, the extent of the dependence seems somewhat stronger in category III than category I.

Figure 5 shows the influence on volatilization of arbitrarily changing the thickness d of the stagnant boundary layer while forcing evaporation to be either 0 or 2.5 mm/d. This arbitrary action has the effect of decoupling water evaporation and boundary layer thickness (Eq. [10]), but could be accomplished in prin-

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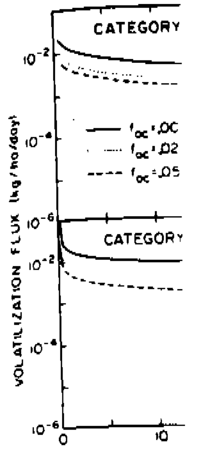

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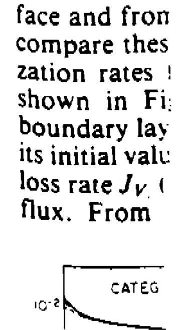

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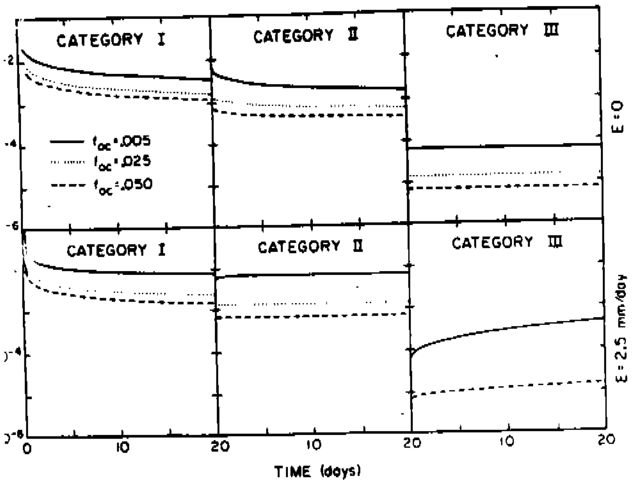

ig. 4—Effect of changes in organic C fraction on volatilization flux rates for the three chemical prototypes. Top curves are for zero evaporation and bottom curves are for evaporation of 2.5 mm/d.

iple by adjusting the relative humidity of the air above he boundary layer so as to maintain E = constant. Here it is obvious that the category I chemical has a olatilization rate that is independent of boundary layer hickness in the range $d < 5$ cm and that the category II chemical has a volatilization rate that is inversely roportional to boundary layer thickness over the range .05 $< d <$ 5 cm.

DISCUSSION

Volatilization without Evaporation

Since Eq. [8] and [9] are respectively the maximum rate of chemical movement through the soil to the surface and from the surface to the air, it is worthwhile to compare these fluxes with the actual predicted volatilization rates for the three chemical categories. This is shown in Fig. 6, where the dashed curve gives the boundary layer flux J_{V_1} (Eq. [9]) where $C_G(o)$ is held at its initial value, the dotted curve gives the maximum soil loss rate J_{V_1} (Eq. [8]) and the solid curve gives the actual flux. From this figure it is clear that the category I chemical behaves as though there is no boundary layer resistance [$C_G(o) = 0$] and the category III chemical behaves as though there is no soil resistance [$C_G(o)$ remains at its initial value]. The category II chemical has properties that create soil and boundary layer resistance of approximately similar size.

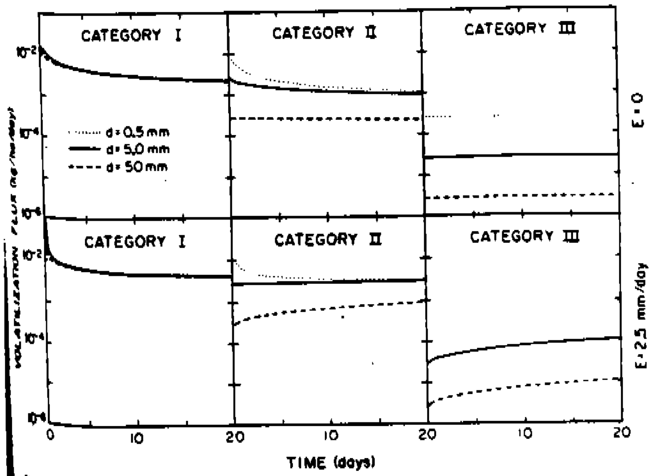

Fig. 5—Effect of changes in diffusion boundary layer thickness on volatilization flux rate for the three chemical prototypes. Top curves are for zero evaporation rate and bottom curves for evaporation of 2.5 mm/d.

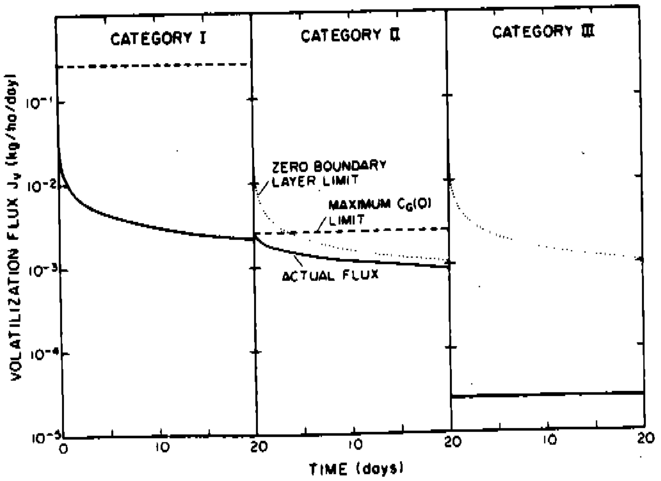

Fig. 6—Calculated volatilization flux rates for the three chemical prototypes when water evaporation is not occurring (solid lines), along with maximum flux through boundary layer given by Eq. [3] (dashed lines) and maximum flux possible when no boundary layer is present, calculated from Eq. [2] (dotted lines).

Thus, Eq. [8] and [9] may be used to represent the volatilization rates of category I and III chemicals, respectively, when no water evaporation is present. In particular, the functional dependence of the volatilization rate on various soil and chemical parameters may be obtained by plugging in the defining equations for D_E and R_G into Eq. [8] and [9], respectively.

Category I Chemicals

$$J_V \propto C_o K_H^{1/2} a^{5/3} K_{oc}^{-1/2} f_{oc}^{-1/2} t^{-1/2} \qquad [18]$$

Category III Chemicals

$$J_V \propto C_o K_H K_{oc}^{-1} f_{oc}^{-1} d^{-1} \qquad [19]$$

Equations [18] and [19] explain the relevant functional dependences of the $E = 0$ volatilization curves shown in Fig. 1–5. For example, Eq. [19] approximately predicts that a category III chemical will have a volatilization rate that has no Θ dependence (Fig. 3), no time dependence (Fig. 3), will be inversely proportional to f_{oc} (Fig. 4), and inversely proportional to d (Fig. 5).

Volatilization with Evaporation

The limiting behavior for volatilization with evaporation is more complex than the evaporation-free case for several reasons. First, both diffusion and convection may contribute to the movement of chemical toward the soil surface. Therefore, category I chemicals will not have volatilization rates that are equal to the rate at which the chemical is moved with water in accordance with Eq. [13], except at large times if the system approaches a steady-state rate of loss. Second, for a boundary-layer limited chemical (category III), upward

Table 3—Theoretical influence of various soil and environmental parameters on pesticide leaching and volatilization rate summarized by chemical category.

Parameter	Category I	Category III
	Convective mobility time, t_c	
Θ	Small, unless $K_{oc} \ll 0.1$ (m³/kg)	Small, unless $K_{oc} \ll 0.1$
f_{oc} (or K_{oc})	f_{oc}	f_{oc}
K_H	None	None
	Volatilization without evaporation	
Θ	$D_G(\Theta)^{1/2}$	None
f_{oc} (or K_{oc})	$f_{oc}^{-1/2}$	f_{oc}^{-1}
K_H	$K_H^{1/2}$	K_H
t	$t^{-1/2}$	None
d	None	d^{-1}
$C_T(o)$	$C_T(o)$	$C_T(o)$
	Volatilization with evaporation	
Θ	$D_G(\Theta)^{1/2}$ for small t; none for large t	Increases as $D_L(\Theta)$ decreases
f_{oc} (or K_{oc})	$f_{oc}^{-1/2}$ for small t; f_{oc} for large t	Increases as f_{oc} decreases
d	None	d^{-1}
t	Decreases as $t^{-1/2}$ to to constant value	Increases as t increases
$C_T(o)$	$C_T(o)$	$C_T(o)$
e	Moderately sensitive for small K_{oc}; insensitive for large K_{oc}	Very sensitive for small K_{oc}

convection can cause concentrations to build up at the surface above the initial value just as salt accumulates at an evaporation surface. In this case, the vapor pressure and vapor density of the chemical at the soil-air boundary can increase with time, limited only by its saturation value. As the vapor density increases, so does the volatilization flux (Eq. [9]). This explains the time dependence shown in Fig. 2 for the category III chemical. As the concentration builds up at the surface, diffusion tends to move chemical back into the soil. Thus, for a given convective flux, the surface concentration at a given time will be highest when the soil diffusion coefficient D_E is lowest. This explains the somewhat strange effect of water content changes on volatilization flux (Fig. 3) predicted to occur for a category III chemical when water evaporation is present. The volatilization flux in Fig. 3 decreases as water content increases. From Fig. 1 we see that D_E increases as water content increases and hence that the surface concentration decreases as water content increases.

Influence of Evaporation on Volatilization

For all three chemical categories, the volatilization rate is enhanced by evaporation (Fig. 2). By comparing the top and bottom curves in Fig. 4, however, it is seen that the extent of the enhancement for a given E decreases as f_{oc} increases. For category I chemicals this is explained by the fact that upward diffusion varies as $f_{oc}^{-1/2}$ (Eq. [18]), whereas upward convection is proportional to C_L, which varies as f_{oc}^{-1}. For large f_{oc}, therefore, convection has a relatively small influence on J_V. For category III chemicals the flux rate is proportional to $C_G(o)$, which remains near its initial value for evaporation-aided volatilization due to upward convection. As f_{oc} increases, the rate of decrease of $C_G(o)$ with time lowers because upward convection decreases. Thus, we may conclude that in all cases evaporation most strongly influences volatilization for weakly adsorbed chemicals with non-negligible vapor density.

SUMMARY AND CONCLUSIONS

Table 3 summarizes the significant functional dependencies for leaching mobility and volatilization of category I and category III chemicals on various soil and environmental parameters found in the simulation studies conducted in this paper. The dependencies shown are for chemicals that clearly fall into the appropriate categories by the criteria given in Eq. [6] or [11]. For category II chemicals, the behavior will in all cases be intermediate between category I and III. Since the model is intended as a screening tool, the functional dependencies given in Table 3 and shown in Fig. 1-5 will help to characterize the susceptibility of a candidate chemical to various loss pathways.

In a future paper we will illustrate the use of the screening model on a number of organic chemicals for which we have obtained benchmark chemical data (Jury et al., 1984a) and will show how these chemicals fall into the groups discussed in this paper. In the final paper in this series (Jury et al., 1984b) we will review the experimental literature to show support for many of the assumptions and predictions of our model.

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