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AP-42 Section 9.2.2
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Behavior Assessment Model for Trace Organics in Soil: III. Application of Screening Model[1]

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ABSTRACT

The soil chemical screening model developed in Jury et al. (1983) is applied to a set of 35 chemicals for which benchmark properties (organic C partition coefficient, vapor pressure, solubility, half-life) have been obtained. Environmental screening tests are conducted on the chemicals to determine their relative convective mobility, diffusive mobility, volatility, and persistence with the results presented in a series of classifications rating the susceptibility of the chemical to a given loss pathway.

The convective mobility tests estimate the time required for a pulse of chemical to travel a distance of 10 cm through an ideal soil of uniform water content and organic C content while being subjected to a water application rate of 1 cm/day. The diffusive mobility tests determine the time required for a chemical to diffuse 10 cm through the same ideal soil. In the volatilization screening tests, each chemical is applied at a uniform concentration of 1 kg/ha to a standard depth in the soil with uniform properties and is allowed to volatilize through a stagnant air boundary layer during a specified time period in the presence or absence of water evaporation. The resulting volatilization fluxes and cumulative losses for a standard time period are used to categorize the relative susceptibility of the chemical to loss to the atmosphere. The persistence tests are used to determine the amount of chemical left after a specified time period when it is free not only to degrade but also to volatilize.

Additional Index Words: **chemical movement, diffusion, volatilization, leaching.**

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There have been a number of reviews written in recent years in which chemical properties have been assembled for a group of organic compounds for the purpose of characterizing environmental behavior. Helling (1971) and Helling et al. (1971) have used thin-layer chromatography to assess the relative mobility of dissolved chemicals during leaching. Their resulting classification of relative mobility is summarized in terms of R_F values of the chemicals; R_F values denote their relative movement along a thin soil layer. They proposed five categories ranging from highly mobile to immobile. Kenaga and Goring (1980) assembled experimental data from 170 chemicals and found a relationship between water solubility, organic C partition coefficient, and soil bioconcentration factors in animal organisms. Rao and Davidson (1980) published a large list of pesticide organic C and octanol-water partition coefficients as well as half-lives for chemicals and provided a series of categories designating persistence based on the half-lives.

In the first two papers of this series (Jury et al., 1983, 1984a), we proposed a general transport model for describing movement through soil in both the liquid and vapor phases for a chemical that partitions between liquid, vapor, and adsorbed phases. The model was developed in order to analyze scenarios in which a given chemical is incorporated uniformly over a finite depth in the soil and is allowed to volatilize with or without the presence of water evaporation. In this paper we will illustrate the use of the model for screening tests on a number of pesticides and other chemicals for which benchmark properties are available. From these results we will attempt to divide the chemicals into general groups, based on their susceptibility to various loss pathways in soil.

DESCRIPTION OF CHEMICALS[3]

Table 1 gives the saturated vapor density, C_G^*; aqueous solubility, C_L^*; organic C partition coefficient, K_{oc}; Henry's constant, K_H; and half-life, $T_{1/2}$, for the 35 chemicals used in our screening tests, together with references for the values used. For several of the chemicals, we had to calculate K_{oc} from the octanol water partition coefficient K_{ow} or from the water solubility regression given in Kenaga (1980). This log-log regression had a $r^2 = 0.79$ when used on the 29 chemicals for which we had both K_{oc} and C_L^* values. Also, for 15 of the chemicals—primarily volatile ones with high vapor pressure—we have not been able to obtain a half-life. In these cases we have conducted our screening tests without allowing these compounds to degrade ($T_{1/2} = \infty$). However, the volatilization rate of these compounds in soil is high enough that it would not be significantly altered by degradation in the early stages when our assessments are made.

Figure 1 groups the 35 chemicals in a quadrant with log of vapor density plotted against log of solubility, both expressed in milligrams per liter. The values plotted correspond to the numbers in Table 1. Also shown are the lines of constant Henry's constant, K_H; they range over almost 11 orders of magnitude in this group of chemicals (from 3.7×10^{-9} for bromacil to 1.4×10^2 for *n*-octane). As discussed in Jury et al. (1984a), K_H values are a very useful index for classifying volatilization behavior.

DESCRIPTION OF SCREENING TESTS

The screening tests performed below are designed to assess relative convective (liquid) mobility, diffusive (primarily as vapor) mobility, susceptibility to loss by volatilization, and persistence. The standard conditions are those described in detail by Jury et al. (1983), i.e., initial chemical application of $M = 1$ kg/ha uniformly distributed to depth L (either 1 or 10 cm) with uniform soil properties (porosity, ϕ; bulk density, ϱ_b; water content, Θ; air content, a; organic C fraction, f_{oc}) and steady water flow, J_W, either upward as evaporation, downward as leaching, or zero.

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[3] See the Appendix for a listing of scientific names of chemicals used in this article.

Table 1—Benchmark properties used for the chemicals in the screening tests. Reference numbers refer to citation number at end of text.

No.	Chemical	Vapor density	Ref. no.	Solubility	Ref. no.	K_{oc}	Ref. no.	$T_{1/2}$	Ref. no.	Henry's constant
		mg/L		mg/L		m³/kg		days		K_H
1	Atrazine	8.0E−0.6†	5	3.2E+0.1	4	1.6E−01	26	71	26	2.5E−07
~~2~~	Benzene	4.0E+02	33	1.8E+03	33	~~8.3E−0.2~~	18	∞‡	-	~~2.2E−01~~
3	Biphenyl	4.9E−01	33	7.5E+00	33	1.4E+00§	18	∞	-	6.6E−02
4	Bromacil	3.0E−06	34	8.2E+02	36	7.2E−02	26	350	26	3.7E−08
5	Bromobenzene	2.8E+00	33	4.5E+02	33	1.5E−01	18	∞	-	6.2E−03
6	Carbofuran	1.0E−04	2	3.2E+02	1	2.8E−02	26	40	26	3.1E−07
~~7~~	Carbon tet.	7.5E+02	33	8.0E+02	33	~~1.1E−01§~~	18	∞	-	~~9.4E−01~~
~~8~~	Chlorobenzene	7.1E+01	33	4.7E+02	33	~~1.5E−01§~~	18	∞	-	~~1.5E−01~~
~~9~~	Chloroform	9.6E+02	33	8.0E+03	33	~~2.9E−02~~	§	∞	-	~~1.2E−01~~
10	2,4-D	5.0E−06	7	9.0E+02	36	2.0E−02	26	15	26	5.6E−09
11	DDT	6.0E−06	29	3.0E−03	9	2.4E+02	26	3837	10	2.0E−03
12	Diazinon	2.0E−03	¶	4.0E+01	18	8.5E−02	26	32	26	5.0E−05
13	Dieldrin	1.0E−04	27	1.5E−01	3	1.2E+01	26	868	23	6.7E−04
14	Diuron	2.0E−06	24	3.7E+01	4	3.8E−01	26	328	26	5.4E−08
15	EPTC	2.2E−01	25	3.7E+02	36	2.8E−01	11	30	23	5.9E−04
16	Ethoprophos	4.5E−03	22	7.5E+02	20	1.2E−01	20	50	20	6.0E−06
~~17~~	Ethylene dibr.	1.2E+02	33	3.4E+03	33	~~4.4E−02~~	18	∞	-	~~3.5E−02~~
18	Lindane	1.0E−03	28	7.5E+02	4	1.3E+00	26	266	26	1.3E−04
19	Mercury	1.5E−02	33	3.0E−0.2	33	4.1E+01	§	∞	-	5.1E−01
~~20~~	Methyl bromide	2.0E+04	33	1.3E+04	33	~~2.2E−02~~	§	∞	-	~~1.5E+00~~
21	Methyl para.	2.5E−04	31	5.7E+01	18	5.1E+00	26	15	26	4.4E−06
22	Monuron	2.0E−06	37	2.6E+02	36	1.8E−01	26	166	10	7.6E−09
23	Napropamide	5.8E−05	36	7.3E+01	36	3.0E−01	6	70	36	7.9E−07
24	Napthalene	1.6E+00	33	3.2E+01	33	1.3E+00	18	∞	-	5.0E−02
25	Nitrobenzene	1.8E+00	33	1.8E+03	33	7.1E−02§	18	∞	-	1.0E−03
~~26~~	*n*-Octane	9.4E+01	33	6.6E−01	33	~~6.8E+00~~	§	∞	-	~~1.4E+02~~
27	Parathion	1.5E−04	31	2.4E+01	18	1.1E+01	26	18	26	6.1E−06
28	Phenanthrene	2.0E−03	33	1.3E+00	33	2.3E+01	18	∞	-	1.6E−03
29	Phenol	5.7E−01	33	8.2E+04	33	2.7E−02	18	∞	-	7.0E−06
30	Phorate	1.6E−02	32	5.0E+01	18	6.6E−01	26	82	26	3.1E−04
31	Prometryne	2.7E−05	5	4.8E+01	18	6.1E−01	26	60	35	5.6E−07
32	Simazine	1.7E−07	5	5.0E+00	4	1.4E−01	26	75	26	3.4E−08
33	Triallate	3.2E−03	8	4.0E+00	15	3.6E+00	15	100	36	7.9E−04
34	Trifluralin	2.0E−03	30	3.0E−01	#	7.3E+00	8	132	26	6.7E−03
~~35~~	Vinyl chloride	8.7E+03	33	9.0E+01	33	~~4.0E−01~~	§	∞	-	~~9.7E+01~~

† E−06 = 10^{-6}, etc. ‡ No value available.

§ Calculated from C^* formula in Kenaga and Goring (1980).

¶ O. Heiber (1976), Ciba-Geigy Ltd., Basel, Switzerland (unpublished personal communication).

R. L. Swann, 1982. Dow Chem. Co., Midland, MI (unpublished personal communication).

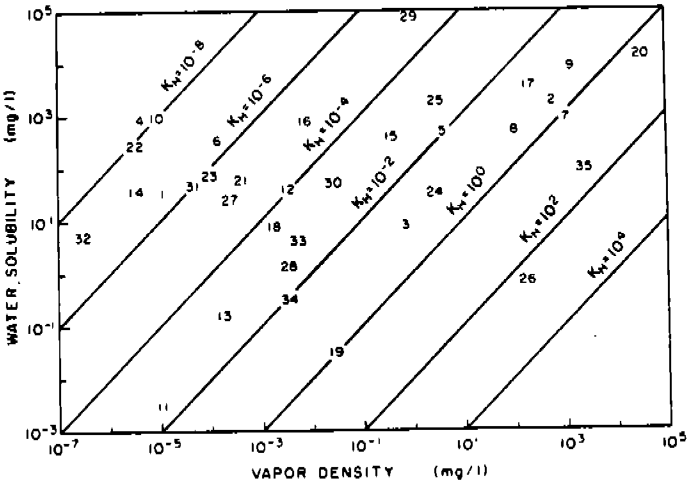

Fig. 1—Vapor density-water solubility plots in milligrams per liter for each of the 35 chemicals. Numbers in the figure correspond to numbers given in Table 1. Solid lines correspond to lines of constant K_H.

Convective Mobility Tests

In order to analyze convective and diffusive mobility in a consistent manner, we will estimate the time required to travel a distance l = 10 cm through the soil by convection and by diffusion, as developed in Jury et al. (1984a). The convective mobility time, t_c, is calculated by assuming piston flow of chemical and instantaneous partitioning between the three phases. The formula, taken from Jury et al. (1984a) is given in Eq. [1]

$$t_c = (\varrho_b f_{oc} K_{oc} + \Theta + aK_H)\, l/J_W. \qquad [1]$$

Diffusive Mobility Tests

The diffusive mobility time, t_D, is small only for vapor-dominated chemicals and is calculated from the formula given in Jury et al. (1984a), summarized here as Eq. [2]

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

where a is volumetric air content and D_G^{air} is the binary gaseous diffusion coefficient in free air.

Volatilization Tests

The simulations of volatilization are conducted using the complete model described in Jury et al. (1983), where each chemical is applied at a uniform concentration of 1 kg/ha to a depth L in the soil and is allowed to volatilize through a stagnant air boundary layer during a specified time period in the presence or absence of water evaporation. The resulting volatilization fluxes and cumulative losses are used to categorize the relative susceptibility to loss to the atmosphere.

Persistence Tests

For a given chemical, dissipation from the soil occurs both by degradation and volatilization. Since persistence is an essential index for characterizing the effectiveness of the chemical as well as its hazard, a dynamic estimate is needed for persistence, in addition to biochemical half-life values. Persistence, as calculated from the scenarios discussed above, will be summarized in the form of effective half-lives, which include both volatilization and degradation. For a given scenario, this dynamic or volatilization half-life, $T^V_{1/2}$, will be calculated as a function of the amount $M(t)$ remaining in the soil after a time t, by solving $M(t) = M(0) \exp(-0.693t/T^V_{1/2})$ for $T^V_{1/2}$, or

$$T^V_{1/2} = -0.693\, t/\ln(M(t)/M(0)), \qquad [3]$$

where $M(0)$ is the initial mass in the soil, ln is the natural logarithm, and $0.693 = \ln(2)$. The rate coefficient μ, discussed in Jury et al. (1983), is defined as $\mu = \ln(2)/T_{1/2}$.

RESULTS

Mobility Tests

Figure 2 shows soil concentrations vs. depth taken at 30 d after leaching at a steady rate J_W = 1 cm/d for three chemicals (DDT, benzene, and bromacil) chosen from Table 1 to represent a range of benchmark properties. These concentrations were calculated with Eq. [24] from Jury et al. (1983). It is clear from this calculation that for two of the chemicals, DDT and bromacil, a simple accounting of the center of mass of the chemical pulse by piston flow would give a good approximation to downward movement by leaching, and Eq. [1] would give a reasonable estimate of the time required to move a given distance by leaching. However, in the case of benzene, movement by vapor diffusion has completely dispersed the pulse during the 30 d of leaching and an estimate of the location of the center of the pulse is all but impossible to make. For this reason, it is useful both to examine the convective and the diffusive mobility of a compound. If the latter is significant, then one might expect behavior such as that seen in Fig. 2 for benzene, and hence that purely convective mobility indices, such as R_F values (Helling, 1971), are not sufficient to describe their movement.

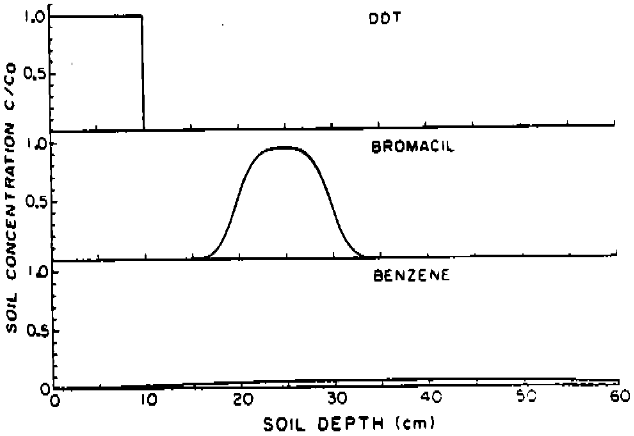

Fig. 2—Pesticide concentration after 30 d of leaching for three representative chemicals using the model of Jury et al. (1983). Standard conditions used are: $\Theta = 0.3, f_{oc} = 0.0125, J_w = 1$ cm/d, $L = 10$ cm.

Table 2 summarizes convective times t_c and diffusive times t_D in days calculated from Eq. [1] and [2], respectively, for the case l = 10 cm and J_W = 1 cm/d. The classification scheme given next to the convective times corresponds to that given in McCall et al. (1980), based on K_{oc} values, where classification 1 represents relatively immobile compounds ($K_{oc} > 5$ m³/kg) and classification 5 represents the most mobile ($K_{oc} < 0.05$ m³/kg). This is similar to the mobility classifications based on R_F values given in Helling (1971). Also shown in Table 2 are the diffusive times that have been qualitatively ranked in a classification scheme where classification 1 represents insignificant diffusive mobility (t_D > 100 d), classification 2 represents moderate mobility ($20 < t_D < 100$), and classification 3 represents high mobility (t_D < 20 d).

By comparing Fig. 2 with Table 2 it is seen that DDT is immobile both in convection (class 1) and diffusion

Table 2—Convection time t_c and diffusion time t_D (days) to travel 10 cm ($\Theta = 0.3, J_W = 1$ cm/d, $f_{oc} = 0.0125$, $\varrho_b = 1350$ kg/m³) along with mobility classification 1-5 (convection) and 1-3 (diffusion).

No.	Chemical	Convection time	Classification	Diffusion time	Classification
		days		days	
1	Atrazine	31	3	–†	1
~~2~~	Benzene	17	4	9	3
3	Biphenyl	239	2	450	1
4	Bromacil	15	4	–	1
5	Bromobenzene	28	4	530	1
6	Carbofuran	8	5	–	1
~~7~~	Carbon tetrachloride	22	4	3	3
~~8~~	Chlorobenzene	28	4	23	2
~~9~~	Chloroform	8	5	8	3
10	2,4-D	6	5	–	1
11	DDT	41 000	1	–	1
12	Diazinon	146	2	–	1
13	Dieldrin	2 043	1	–	1
14	Diuron	68	3	–	1
15	EPTC	51	3	–	1
16	Ethoprophos	24	4	–	1
~~17~~	Ethylene dibromide	10	5	37	2
18	Lindane	222	2	–	1
19	Mercury	6 930	1	–	1
~~20~~	Methyl bromide	7	5	1	3
21	Methyl parathion	864	1	–	1
22	Monuron	34	3	–	1
23	Napropamide	53	3	–	1
24	Napthalene	222	2	550	1
25	Nitrobenzene	15	4	–	1
~~26~~	*N*-octane	1 156	1	1	3
27	Parathion	1 800	1	–	1
28	Phenanthrene	3 884	1	–	1
29	Phenol	8	5	–	1
30	Phorate	114	3	–	1
31	Prometryne	107	2	–	1
32	Simazine	26	4	–	1
33	Triallate	611	1	–	1
34	Trifluralin	1 242	1	–	1
~~35~~	Vinyl chloride	70	3	1	3

† t_D > 1000 d.

(class 1), whereas bromacil is very mobile by convection (class 4) but immobile by diffusion (class 1). For this reason, the pulse of bromacil shown in Fig. 2 moves into the soil but does not significantly change its shape over time. Benzene is also in convection class 4, and by that criterion alone should behave similarly to bromacil. However, benzene has a high diffusive mobility (class 3) and hence penetrates far deeper into the soil than expected based on convection alone. Figure 2 shows how misleading a traditional mobility classification such as the R_F system would be for compounds such as benzene with class 3 diffusive mobility.

Volatilization Tests

Figure 3, 4, and 5 show volatilization fluxes vs. time for each of the 35 compounds for the case of no evaporation (solid curve), evaporation at 2.5 mm/d (dotted curve), and evaporation at 5 mm/d (dashed curve). All of these tests were conducted for standard soil and initial conditions ($M(0) = 1$ kg/ha, $\Theta = 0.3$, $\varrho_b = 1350$ kg/m^3, $f_{oc} = 0.0125$, $L = 10$ cm), and included the stagnant air boundary layer of thickness d through which chemical and water vapor must diffuse to the atmosphere (Jury et al., 1983). The boundary layer thicknesses for the three water evaporation (E) rates, calculated using Eq. [28] of Jury et al. (1983), were $d = 4.75 \times 10^{-3}$ m ($E = 0$ and 2.5 mm/d) and $d = 2.38 \times 10^{-3}$ ($E = 5$ mm/d). Figure 3 contains the so-called volatilization category II and III compounds ($K_H \leq 2.5 \times 10^{-5}$) as discussed in Jury et al. (1983), Fig. 4 contains category I compounds for which evaporation influences volatilization, and Fig. 5 contains category I compounds for which evaporation does not influence volatilization.

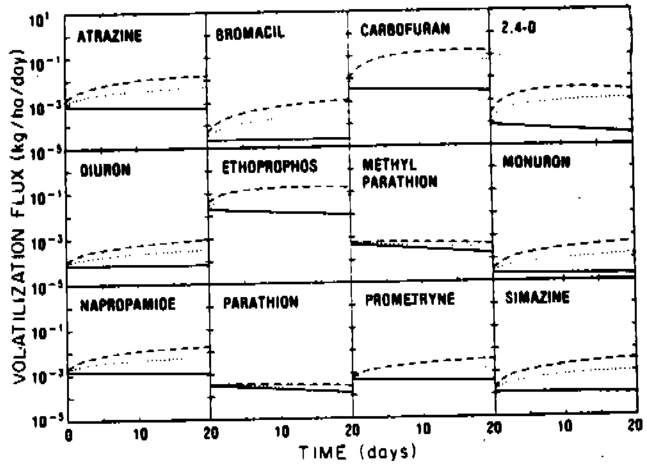

Fig. 3—Volatilization flux vs. time for chemicals used in the screening test. Standard conditions used are: $f_{oc} = 0.0125$; $\Theta = 0.3$; $L = 10$ cm; $E = 0$ (solid curve), $E = 2.5$ mm/d (dotted curve), and $E = 5.0$ mm/d (dashed curve).

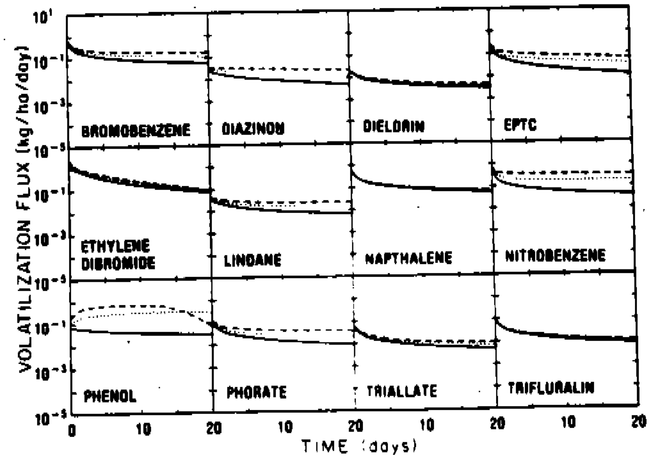

Fig. 4—Volatilization flux vs. time for chemicals used in the screening test. Standard conditions used are: $f_{oc} = 0.0125$; $\Theta = 0.3$; $L = 10$ cm; and $E = 0$ (solid curve), $E = 2.5$ mm/d (dotted curve), and $E = 5.0$ mm/d (dashed curve).

When grouped in this way the compounds follow a consistent behavior pattern, with the volatilization flux of category II and III compounds increasing when evaporation is present, decreasing somewhat with time when volatilization occurs without evaporation. Furthermore, for compounds in category I, volatilization flux decreases with time for all cases. The compounds in Fig. 4 and 5 may be distinguished by whether or not evaporation-aided volatilization is increased significantly relative to volatilization without evaporation.

Persistence Tests

Table 3 gives the mass remaining at 30 d expressed as a percent of the mass initially present for the low volatility compounds, subject to either $E = 0$ or $E = 5$ mm/d and for shallow ($L = 1$ cm) or deep ($L = 10$ cm) incorporation. These results were calculated by integrating Eq. [25] of Jury et al. (1983) and thus include degradation as well as volatilization losses. Table 4 presents percent mass remaining after only 1 d of volatilization for the high volatility compounds in Table 1 for the case of $E = 0$ and $L = 1$ and 10-cm depths of incorporation. Also shown in this table are effective volatilization half-lives, $T^V_{1/2}$, calculated using Eq. [3] for $t = 1$ d. As noted in Table 1, these compounds were assigned infinite degradation half-lives; thus, the $T^V_{1/2}$ values in Table 4 are only for volatilization. Finally, Table 5 calculates effective volatilization half-lives for all of the 35 compounds without evaporation using Eq. [3] and the values given in Table 3 and 4 for $E = 0$ and

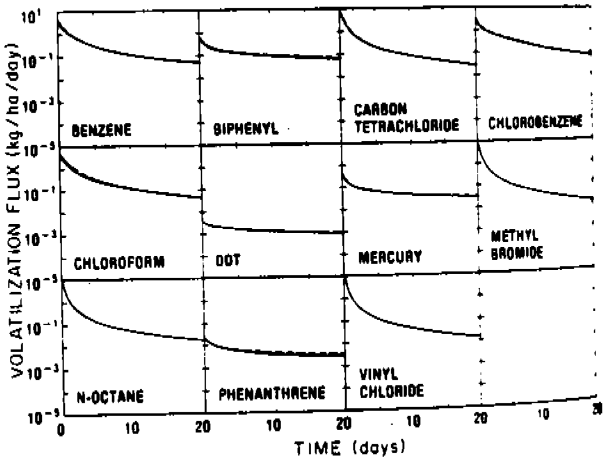

Fig. 5—Volatilization flux vs. time for chemicals used in the screening test. Standard conditions used are: $f_{oc} = 0.0125$; $\Theta = 0.3$; $L = 10$ cm; $E = 0$ (solid curve), $E = 2.5$ mm/d (dotted curve), and $E = 5.0$ mm/d (dashed curve).

Table 3—Percent mass remaining in soil after 30 d of volatilization for low volatility compounds as a function of E (mm/day) and L (cm) along with effective volatilization half-lives (day) calculated from Eq. [3]. ($\Theta = 0.3$, $M(0) = 1$ kg/ha, $f_{oc} = 0.0125$).

	$L = 1$ cm				$L = 10$ cm			
	$E = 0.0$		$E = 5.0$		$E = 0.0$		$E = 5.0$	
Chemical	%	$T^V_{1/2}$	%	$T^V_{1/2}$	%	$T^V_{1/2}$	%	$T^V_{1/2}$
Atrazine	73.6	68	54.6	34	74.7	71	68.5	56
Bromacil	94.3	354	93.3	300	94.3	354	93.8	325
Carbofuran	56.6	37	11.6	10	59.3	40	17.9	12
2,4-D	25.4	15	24.6	15	25.5	15	24.8	15
DDT	95.9	497	95.3	432	99.1	2300	99.0	2069
Diazinon	37.4	21	8.6	8	51.1	31	47.1	28
Dieldrin	85.2	130	80.6	96	96.4	567	95.9	497
Diuron	93.8	330	91.9	246	93.9	330	93.6	314
EPTC	17.9	12	1.9	5	45.9	27	34.7	20
Ethoprophos	45.4	26	0.6	4	63.5	46	27.6	16
Lindane	65.5	49	27.9	16	89.8	193	85.4	132
Methyl parathion	25.2	15	24.1	15	25.4	15	25.3	15
Monuron	88.3	167	87.7	158	88.4	169	88.2	166
Napropamide	72.0	63	43.5	25	74.3	70	68.3	55
Parathion	31.7	18	31.1	18	32.0	18	31.9	18
Phenanthrene	88.5	171	86.5	143	98.9	1799	98.6	1526
Phorate	42.1	24	7.3	8	74.0	69	66.6	51
Prometryne	70.1	59	60.4	41	70.9	60	69.7	58
Simazine	75.9	75	72.2	64	76.0	76	74.8	72
Triallate	60.4	41	48.4	29	79.3	90	78.1	84
Trifluralin	51.7	32	46.6	27	82.1	105	81.5	102

$L = 10$. Table 5 presents a persistence classification scheme ranging from 1 (very persistent) to 5 (very short-lived).

DISCUSSION

Mobility Tests

For compounds that move primarily in the liquid phase, the organic C partition coefficient, K_{oc}, appears to be a useful benchmark property for characterizing susceptibility to leaching. However, for volatile compounds such as fumigants, which have a substantial activity in the vapor phase, movement by vapor diffusion may be significant compared with convective transport. For this reason, it is recommended to use both convective and diffusive criteria for assessing mobility, since, as shown in Fig. 2, convective mobility is not a sufficient criteria for determining movement of benzene or other compounds of high K_H and low K_{oc}. On the other hand, for the high volatility compounds with substantial vapor mobility, dissipation to the atmosphere will be extremely rapid except in those cases where continuous downward movement or a soil cover prevents escape through the soil surface.

Volatility Tests

The similar volatilization behavior of the compounds in category II or III shown in Fig. 3 is consistent with the generalizations given by Jury et al. (1984a). The only compounds in this group for which volatilization decreases with time are those in category II whose biochemical half-lives (parathion, methyl parathion) are short enough to cause substantial disappearance of the compound during the 20 d of simulation. For the rest of the compounds, the dependence of volatilization on evaporation of water is substantial and leads to increases in volatilization flux of up to 2 orders of magnitude at the end of 20 d compared with evaporation-free volatilization.

Table 4—Percent mass remaining in soil and effective volatilization half-life (days) after 1 d of volatilization without water evaporation ($\Theta = 0.3$, $M(0) = 1$ kg/ha, $f_{oc} = 0.0125$) for high volatility compounds.

	Percent remaining		Half-life $T^V_{1/2}$	
Chemical	$L = 1$ cm	$L = 10$ cm	$L = 1$ cm	$L = 10$ cm
Benzene	8.7	63.0	0.3	1.6
Biphenyl	50.4	94.6	1.0	12.6
Bromobenzene	52.6	94.5	1.1	13.4
Carbon tetrachloride	4.9	44.0	0.2	0.8
Chlorobenzene	13.5	76.6	0.3	12.6
Chloroform	8.1	61.6	0.3	1.4
Ethylene dibromide	16.8	81.4	0.4	3.4
Mercury	72.4	97.3	2.1	24.7
Methyl bromide	2.6	24.4	0.2	0.5
Naphthalene	54.2	95.2	1.1	14.0
Nitrobenzene	65.4	96.5	1.6	19.4
N-octane	3.2	29.9	0.2	0.6
Phenol	67.6	96.8	1.8	20.9
Vinyl chloride	2.5	24.2	0.2	0.5

Table 5—Persistence classes defined in terms of effective half-life $T^{V_{1/2}}$ (days) under standard conditions of deep placement ($L = 10$ cm, $\Theta = 0.3$, $E = 0$).

Herbicide	$T^V_{1/2}$	Herbicide	$T^V_{1/2}$
	days		days
Class 1. Highly persistent $T^V_{1/2} > 100$			
Bromacil	354	Lindane	193
DDT	2300	Monuron	169
Dieldrin	567	Phenanthrene	1799
Diuron	330	Trifluralin	105
Class 2. Moderately persistent $30 < T^V_{1/2} < 100$			
Atrazine	71	Phorate	69
Carbofuran	40	Prometryne	60
Diazinon	31	Simazine	76
Ethoprophos	46	Triallate	90
Napropamide	70		
Class 3. Moderately short-lived $15 < T^V_{1/2} < 30$			
2,4-D	15	Nitrobenzene	19
EPTC	27	Parathion	18
Methyl parathion	15	Phenol	21
Mercury	25		
Class 4. Short-lived $5 < T^V_{1/2} < 15$			
Biphenyl	13	Chlorobenzene	13
Bromobenzene	13	Napthalene	14
Class 5. Very short-lived $T^V_{1/2} < 5$			
Benzene	1.6	Ethylene dibromide	3.4
Carbon tetrachloride	0.8	Methyl bromide	0.5
Chloroform	1.4	*N*-octane	0.6
		Vinyl chloride	0.5

The category I compounds shown in Fig. 4 and 5 also behave consistently and differ only in the extent of dependence on evaporation. As discussed in Jury et al. (1984a), enhancement of volatilization flux by evaporation depends primarily on the relative importance of upward movement to the soil surface by convection and vapor diffusion to the atmosphere at the soil surface. Thus, those compounds in Fig. 5 with large K_{oc} (i.e., large t_c) (biphenyl, DDT, mercury, *n*-octane, and phenanthrene) will have a small convective flux toward the surface and hence little effect of evaporation on pesticide loss. However, the rest of the compounds in Fig. 5 that show little effect of evaporation on volatilization have small K_{oc}'s. These remaining compounds have very high volatilization fluxes, which are dominated by diffusive loss. Furthermore, the extent of upward convection is controlled by the rapid decrease in initial pulse size by vapor diffusion, since all of the remaining compounds in Fig. 5 have high diffusive mobility (Table 2). It is instructive in this regard to compare the volatilization flux vs. time graphs for chloroform (Fig. 5) and nitrobenzene (Fig. 4). Under evaporation-free conditions, the chloroform volatilization flux is much larger than that of nitrobenzene, except for long time periods. For evaporation-aided volatilization, however, the nitrobenzene flux exceeds that of chloroform after about 4 d when E = 5.0 mm/d. The compounds have two major differences. Nitrobenzene has negligible vapor diffusion (vapor mobility class 1), whereas chloroform has high (class 3) vapor diffusive mobility. Thus, the nitrobenzene pulse will approximately retain its initial shape during volatilization, so that the liquid concentration moving to the surface by convection is high. Chloroform, on the other hand, will diffuse downward and the pulse will decrease in size much as benzene did during leaching in Fig. 2. As a consequence, the equilibrium liquid concentration moving to the surface by convection is smaller than that of nitrobenzene, even though their liquid partition coefficients, $R_L = C_T/C_L$, where C_T is total concentration and C_L is solution concentration, are similar. Hence, evaporation does not enhance the volatilization of compounds like chloroform.

Persistence Tests

Tables 3 to 5 demonstrate that volatility can greatly affect the persistence of many of the compounds screened. In fact, Table 5 suggests that many of the degradation coefficient measurements made in the field have probably been influenced by volatilization losses and hence are not a good index of biochemical activity. For persistence class 1 compounds, shallow placement greatly influences effective half-life and persistence. For example, lindane was calculated to have an effective volatilization half-live of $T^V_{1/2}$ = 49 d with 1-cm placement and 193 d with 10-cm placement (E = 0). Furthermore, these effective volatilization half-lives are greatly reduced (to 16 and 132 d, respectively) when water evaporation is present. Our benchmark degradation half-life for lindane (Table 1), based on laboratory measurements with volatilization suppressed, is 266 d. For shallow placement, the degradation loss pathway is insignificant compared with volatilization. On the other hand, monuron, which does not volatilize significantly, has essentially the same effective half-life ($T^V_{1/2}$ = 266) under all conditions except when E = 5 mm/d and L = 1 cm, when it reduces somewhat to 158 d.

On the basis of information given in Tables 3 and 4, it is possible to group the 35 compounds into qualitative persistence classes. This is done in Table 5, for the standard condition of L = 10 cm, f_{oc} = 0.0125, E = 0, Θ = 0.3. In all cases, the results of these tests are a function of the standard conditions assumed. If the tests were repeated under different organic C fractions, different water contents, etc., somewhat different conclusions might be drawn. However, the analysis of Jury et al. (1984a) was intended to discern the underlying functional dependence of volatilization category I and category III compounds on these standard conditions so that repeated screening tests need not be run in all cases. Thus, for example, using Table 3 of Jury et al. (1984a), one would predict for volatilization flux an inverse dependence on organic C fraction for category III compounds (J_V proportional to f_{oc}^{-1}) and an inverse square root dependence for category I compounds (J_V proportional to $f_{oc}^{-1/2}$) when volatilization occurs without evaporation. Under these conditions, one would also expect no water content dependence for volatilization of category III compounds.

SUMMARY AND CONCLUSIONS

Using the model of Jury et al. (1983), we have performed tests on the 35 chosen chemicals to determine relative convective and diffusive mobility, susceptibility to volatilization at the soil surface, and general persistence in soil as a function of depth of incorporation. The results have been presented in a series of relative categories for susceptibility to loss through the various pathways. This information might be useful in a specific application by considering several different classifications simultaneously, such as convective mobility and persistence to determine whether the chemical will persist long enough to be a hazard to underlying groundwater in an area where leaching is prevalent. Furthermore, information on relative volatility as a function of depth of incorporation is useful for placement design. Finally, if a substantial amount of experimental information is available about the behavior of one compound under natural conditions, this information could serve to represent a group of compounds that have been classified as similar using the screening model. In this manner, the ideal scenarios represented in our model could be linked to the nonideal properties of the real world environment through experimental data.

However, it must be emphasized that this is not a simulation model. The purpose of the series of papers is to present a simple procedure for determining the relative behavior of chemicals under prototype conditions. In the final paper in this series, Jury et al. (1984b), we will review the experimental literature to substantiate the general model assumptions used in the paper and will demonstrate where predicted behavior is manifested and certain trends seen under natural conditions.

APPENDIX

Scientific names of chemicals used in this article.

Common or trade name	Chemical name
Atrazine	2-chloro-4-(ethylamino)-6-(isopropylamino)-*s*-triazine
Bromacil	5-bromo-3-*sec*-butyl-6-methyluracil
Carbofuran	2,3-dihydro-2,2-dimethyl-7-benzofuranylmethylcarbamate
Chloroform	trichloromethane
2,4-D	(2,4-dichlorophenoxy) acetic acid
DDT	1,1,1-trichloro-2,2-bis(*p*-chlorophenyl) ethane

iazinon	*O,O*-diethyl-*O*-(2-isopropyl-6-methyl-4-pyrimidinyl) phosphorothioate
ieldrin	1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a, octahydro-1,4-*endo-exo*-5,8-dimethanonaphthalene
iuron	3-(3,4-dichlorophenyl)-1,1-dimethylurea
PTA	*S*-ethyl dipropylthiocarbamate
thoprophos	*O*-Ethyl *s,s*-dipropyl phosphorodithioate
indane	γ-1,2,3,4,5,6-hexachlorocyclohexane
ethyl parathion	*O,O*-dimethyl *O*-(*p*-nitrophenyl) phosphorodithioate
onuron	3-(*p*-chlorophenyl)-1,1-dimethylurea
apropamide	2-(*a*-naphthoxy)-*N,N*-diethylpropionamide
arathion	*O,O*-diethyl *O*-(*p*-nitrophenyl) phosphorodithioate
horate	*O,O*-diethyl *s*-[(ethylthio) methyl] phosphorodithioate
rometryne	2,4-bis(isopropylamino)-6-methylthio-*s*-triazine
mazine	2-chloro-4,6-bis (ethylamino)-*s*-triazine
riallate	*S*-(2,3,3-trichloroally)diisopropylthiocarbamate
rifluralin	α,α,α-trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine

REFERENCES

. Bowman, B. T., and W. W. Sans. 1979. The aqueous solubility of twenty-seven insecticides and related compounds. J. Environ. Sci. Health 14B:625-634.

. Cook, R. F. 1973. Carbofuran. p. 187-210. *In* G. Zweig (ed.) Analytical methods for pesticides and plant growth regulators. Academic Press, New York.

. Eye, J. D. 1968. Aqueous transport of dieldrin residues in soils. J. Water Pollut. Control Fed. 40:R316-R332.

. Freed, V. H. 1976. Solubility, hydrolysis, dissociation constants and other constants of benchmark pesticides. p. 1-18. *In* Literature survey of benchmark pesticides. George Washington University Medical Center, Washington, DC.

. Friedrich, K., and K. Stammbach. 1964. Gas chromatographic determination of small vapour pressures. Determination of the vapour pressures of some triazine herbicides. J. Chromatogr. 16:22-28.

6. Gerstl, Z., S. Saltzmann, L. Kliger, and B. Yaron. 1981. Distribution of herbicides in soil in a simulated drip irrigation system. Irrig. Sci. 2:155-166.

7. Goring, C. A. I. 1967. Physical aspects of soil in relation to the action of soil fungicides. Annu. Rev. Phytopathol. 5:285-318.

. Grover, R., W. F. Spencer, W. J. Farmer, and T. D. Shoup. 1978. Triallate vapor pressure and volatilization from glass surfaces. Weed Sci. 26:505-508.

9. Gunther, F. A., W. E. Westlake, and P. S. Jaglan. 1968. Reported solubilities of 738 pesticide chemicals in water. Residue Rev. 20:1-148.

0. Hamaker, J. W. 1972. Decomposition: quantitative aspects. p. 253-340. *In* C. A. I. Goring and J. W. Hamaker (ed.) Organic chemicals in the soil environment. Marcel Dekker, Inc., New York.

1. Hamaker, J. W., and J. M. Thompson. 1972. Adsorption. p. 49-144. *In* C. A. I. Goring and J. W. Hamaker (ed.) Organic chemicals in the soil environment. Marcel Dekker, Inc., New York.

2. Helling, C. S. 1971. Pesticide mobility in soils: III. Influence of soil properties. Soil Sci. Soc. Am. J. 35:743-748.

13. Helling, C. S., P. C. Kearney, and M. Alexander. 1971. Behavior of pesticides in soils. Adv. Agron. 23:147-240.

14. Jury, W. A., W. J. Farmer, and W.F. Spencer. 1984a. Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. J. Environ. Qual. 13:567-572 (this issue).

15. Jury, W. A., R. Grover, W. F. Spencer, and W. J. Farmer. 1980. Modeling vapor losses of soil-incorporated triallate. Soil Sci. Soc. Am. J. 44:445-450.

16. Jury, W. A., W. F. Spencer, and W. J. Farmer. 1983. Behavior assessment model for trace organics in soil: I. Model description. J. Environ. Qual. 12:558-564.

17. Jury, W. A., W. F. Spencer, and W. J. Farmer. 1984b. Behavior assessment model for trace organics in soil: IV. Review of experimental evidence. J. Environ. Qual. 13:580-586 (this issue).

18. Kenaga, E. E. 1980. Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. Ecotoxicol. Environ. Saf. 4:26-38.

19. Kenaga, E. E., and C. A. I. Goring. 1980. Relationship between water solubility, soil sorption octanol-water partitioning, and bioconcentration of chemicals in biota. *In* J. C. Eaton (ed.) Aquatic toxicology ASTM STP 707. American Society for Testing and Materials, Philadelphia, PA.

20. Liestra, M. 1979. Computing the movement of ethoprophos in soil after application in spring. Soil Sci. 128:303-311.

21. McCall, P. J., R. L. Swann, D. A. Laskowski, S. M. Unger, S. A. Vrona, and H. J. Dishburger. 1980. Estimation of chemical mobility in soil from liquid chromatographic retentatives. Bull. Environ. Contam. Toxicol. 24:190-195.

22. Mobil Chemical Co. 1973. "MOCAP," Technical Bulletin. Mobil Chemical Company, Richmond, VA.

23. Nash, R. G. 1980. Dissipation rate of pesticides from soils. p. 560-594. *In* W. G. Knisel (ed.) CREAMS. Vol. 3. U.S. Department of Agriculture, Washington, DC.

24. Nex, R. W., and A. W. Swezey. 1954. Some chemical and physical properties of weed killers. Weeds 3:241-253.

25. Patchett, G. G., G. H. Batchelder, and J. J. Menn. 1964. Eptam. p. 117-123. *In* G. Zweig (ed.) Analytical methods for pesticides, plant growth regulators, and food additives. Vol. IV. Academic Press, New York.

26. Rao, P. S. C., and J. M. Davidson. 1980. Estimation of pesticide retention and transformation parameters required in nonpoint source pollution models. p. 23-67. *In* M. R. Overcash and J. M. Davidson (ed.) Environmental impact of nonpoint source pollution. Ann Arbor Science Publishers, Inc., Ann Arbor, MI.

27. Spencer, W. F., and M. M. Cliath. 1969. Vapor density of dieldrin. Environ. Sci. Technol. 3:670-674.

28. Spencer, W. F., and M. M. Cliath. 1970. Desorption of lindane from soil as related to vapor density. Soil Sci. Soc. Am. Proc. 34: 574-578.

29. Spencer, W. F., and M. M. Cliath. 1974. Factors affecting loss of trifluralin from soil. J. Agric. Food Chem. 22:987-991.

30. Spencer, W. F., and M. M. Cliath. 1982. Volatility of DDT and related compounds. J. Agric. Food Chem. 20:645-649.

31. Spencer, W. F., T. D. Shoup, M. M. Cliath, W. J. Farmer, and R. Haque. 1979. Vapor pressures and relative volatility of ethyl and methyl parathion. J. Agric. Food Chem. 27:273-278.

32. Sutherland, G. L., P. A. Giang, and T. E. Archer. 19 . Thimet. p. 487-505. *In* G. Zweig (ed.) Analytical methods for pesticides, plant growth regulators and food additives. Vol. II. Academic Press, New York.

33. Thomas, R. G. 1982. Volatilization from water. p. 15-1-15-34. *In* W. J. Lyman et al. (ed.) Handbook of chemical property estimation methods—environmental behavior of organic compounds. McGraw-Hill Book Company, New York.

34. U.S. Environmental Protection Agency. 1975. Substitute chemical program—initial scientific and minieconomic review of bromacil. USEPA Rep. 540/1-75-006. U.S. Government Printing Office, Washington, DC. p. 14.

35. Wauchope, R. D. 1978. The pesticide content of surface water draining from agricultural fields—a review. J. Environ. Qual. 7: 459-472.

36. Weed Science Society of America. 1974. Herbicide handbook. 3rd ed. Weed Science Society of America, Champaign, IL.

37. Wiedemann, H. G. 1972. Applications of thermogravimetry for vapor pressure determination. Thermochim. Acta 3:355-356.