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Project Summary

Treatment Potential for 56 EPA Listed Hazardous Chemicals in Soil

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The full report presents information on the quantitative evaluation of the treatment potential in soil for 56 substances identified as hazardous by the U.S. Environmental Protection Agency (EPA). The 56 chemicals evaluated were organized into four categories of substances: (1) polynuclear aromatic hydrocarbons (PAH), (2) pesticides, (3) chlorinated hydrocarbons, and (4) miscellaneous chemicals. Treatability screening studies were conducted to determine: (1) degradation rates, (2) partition coefficients among air, water, soil, and oil phases, and (3) transformation characteristics. The quantitative information developed for a subset of the tested chemicals was input into two mathematical models specifically adapted to describe the treatment process. Results of fate and transport predictions of the models were compared with laboratory and literature results in order to evaluate the ability of the models to predict the behavior of the selected chemicals in a soil system.

The experimental approach used in this study was designed to characterize degradation, immobilization, and transformation potentials for the hazardous substances evaluated. Biodegradation rates were determined experimentally by applying the chemical of interest to a soil microcosm and monitoring concentration over time. A plot of the disappearance of a constituent versus treatment time provided the following information: (1) reaction rate constant, and (2) half-life in soil (first order reaction assumed). Special methods were employed to determine biodegradation rates corrected for volatilization losses for the constituents tested. Losses were also determined in microbially inactive soil/substance controls for a subset of substances to indicate contribution to degradation of abiotic (e.g., hydrolysis, oxidation, etc.) processes. Transport data were developed using calculational procedures based on structure-activity relationships (SARs). To determine partition coefficients among soil, air, oil, and water phases one set of studies was conducted using the radiolabeled compound 7,12-dimethylbenz-(a)anthracene (DMBA) in order to evaluate the potential for formation of biochemical intermediates during the biodegradation of DMBA, and to determine the extent of incorporation of the chemical into soil organic matter. Treatability data generated in this investigation were entered into the Soil Transport and Fate Data Base developed as part of a concurrent EPA-funded study.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Biodegradation is believed to be the most important degradative mechanism for organic compounds in soil and is utilized in soil treatment systems for the

transformation of hazardous organic chemicals into innocuous products. The primary goal of biodegradation testing is to obtain an overall estimate of the rate at which a compound will biodegrade in a soil environment. For quantitative assessment of the rate of biodegradation of an individual constituent in a soil system, it is necessary to measure: (1) changes in parent compound concentration with time, (2) loss of chemical due to volatilization, and (3) chemical loss due to abiotic mechanism. In addition to the degradation of hazardous constituents, the immobilization (related to partitioning into solid, liquid, and gaseous phases) and the transformation of parent compounds to intermediate products within a soil system represent additional information requirements for assessing the potential for treatment of hazardous constituents in soil.

The information generated in this study was input into a comprehensive Soil Transport and Fate Data Base that has been established to address the behavior of hazardous substances in soil systems. Specific quantitative information concerning persistence and/or partitioning for 56 substances was developed to provide EPA with an information base for use in making decisions concerning the treatability of the tested chemicals in soil.

Specific objectives of this research project were to:

1. Determine degradation kinetic information corrected for volatilization.

2. Determine the extent of chemical incorporation into soil organic material, and the biological and chemical characterization of transformation products.

3. Determine the contribution of. abiotic loss to "apparent loss rates."

4. Determine partition coefficients among oil, water, air, and soil phases.

5. Input the data generated for degradation rates and partition coefficients for a subset of the substance evaluated into the RITZ and VIP mathematical models to evaluate the potential terrestrial transport and fate of the substances in soil systems.

Research Approach

Substances evaluated—Four categories of 56 substances were evaluated: (1) polynuclear aromatic hydrocarbons (PAHs), (2) pesticides, (3) chlorinated hydrocarbons, and (4) miscellaneous substances.

All chemicals except toxaphene and tetraalkyllead (TAL) were purchased commercially, analytical grade. The toxaphene sample was collected from a soil site where spent toxaphene cattle dipping solution had been disposed. The TAL sample was provided by Standard Oil of California, and consisted of tetraalkyllead (61.5%), ethylene dibromide (17.9%), and ethylene dichloride (18.8%).

Soils evaluated—Two soils were used in this study, a Kidman fine sandy loam (Haplustoll, Utah) and a McLaurin sandy loam soil (Paleudult, Mississippi). Neither soil had received application of any fertilizer or agricultural chemical in the last five years. Soil microorganism counts were typical for a soil with an active microbial population.

Determination of degradation rates in soil—Degradation describes the chemical and/or biological conversion of a parent compound to its various intermediates and/or to inorganic end products such as carbon dioxide, water, nitrogen, phosphorous, sulfur, etc. In this study, the rate of degradation was experimentally determined by measuring the difference between the amount of compound initially added to a soil and that which was recovered after specified time intervals. Biological and chemical degradation components were differentiated using control soil samples treated with $HgCl_2$. This operational determination of degradation, however, did not distinguish between complete degradation and transformation into intermediate products.

Two experimental approaches were used to measure degradation rates for the chemicals evaluated in the study. In the first approach the observed loss of a compound due to volatilization was not distinguished from losses attributed to degradation rates. In the second approach, degradation rates were corrected for volatilization. The later approach involved independent measurement of losses due to volatilization thus allowing a corrected degradation rate for volatile chemicals to be determined.

Partition Coefficient Determinations— Partition coefficients between aqueous

and soil (K_d) oil (K_o), and air (K_h) phases were estimated based on structure-activity relationships using the following methods.

The partition coefficient of a chemical between soil and water (K_d) is given by:

$$K_d = C_s/C_w \qquad (1)$$

where K_d is the soil/water partition coefficient (unitless if C_s and C_w are in the same units), C_s is the concentration of chemical in the soil phase, and C_w is the concentration of chemical in the aqueous phase.

K_d values for a soil can be estimated from K_{oc} values if the organic fraction of the soil, f_{oc}, is known and if it is assumed that hydrophobic interactions dominate the partitioning process:

$$K_d = K_{oc}f_{oc} \qquad (2)$$

where K_{oc} is the organic carbon normalized soil/water partiion coefficient.

By assuming that partitioning between water and the organic fraction of soil is similar to partitioning between octanol and water, several correlation equations have been developed which relate K_{oc} to octanol/water partition coefficients (K_{ow}). The correlation equation used to calculate K_{oc} for this project was:

$$\log K_{oc} = 1.0 \log K_{ow} - 0.21 \qquad (3)$$

Experimental values of $\log K_{ow}$ obtained from the literature were used when available. Log K_{ow} values, estimated using the fragment approach of Hansch and Leo, were used when experimental values were not available.

The second approach employed for the estimation of $\log K_{oc}$ was based on molecular connectivity indexes (MCIs). MCIs are topological parameters that describe the degree of bonding or connectedness of the nonhydrogen atoms in a molecule. First-order MCIs (^1x), calculated from the molecular structure of a compound, have been shown to be highly correlated with soil/water partition coefficients.

First order MCIs were calculated using a computer program written in Fortran for an Apple Macintosh computer. The K_{oc} values were calculated from the first order MCI using the regression equation:

$$\log K_{oc} = (0.53) \, ^1x + 0.54 \qquad (4)$$

The resultant K_{oc} values were used along with percent organic carbon values to calculate K_d values of the Kidman and McLaurin soils using equation 2.

The pattern coefficient of a chemical between water and oil (K_d) is given by:

$$K_o = C_o/C_w \quad (5)$$

where K_o is the oil/water partition coefficient (unitless if C_o and C_w are in the same units), C_o is the concentration of chemical in the oil phase, and C_w is the concentration of chemical in the water phase.

K_o values were estimated using a correlation expression between K_o and K_{ow} and are presented below:

$$\log K_o = 1.12 \log K_{ow} - 0.324 \quad (6)$$

The partition coefficient of a chemical between air and water (K_h) can be written as:

$$K_h = C_a/C_w \quad (7)$$

where K_h is the air/water partition coefficient, C_a is the concentration of chemical in the air phase, and C_w is the concentration of chemical in the aqueous phase.

K_h can also be expressed as a dimensionless Henry's Law constant H/RT. Values of H can be calculated from the ratio of vapor pressure of a chemical to aqueous solubility if it is assumed that the liquid phase activity coefficients are constant up to the solubility limit. Using experimental values for vapor pressure (P_v) and aqueous solubility (S) obtained from the literature, K_h was calculated using the following expressions:

$$K_h = H/RT = (P_v/S)/RT \quad (8)$$

where P_v is the vapor pressure (torr), S is aqueous solubility (moles/liter), R is the gas constant (62.3 liter torr/atm K) and T is temperature (25°C, 298°K).

If literature values of P_v or S were unavailable for a particular compound but boiling point and melting point values were available, P_v values were estimated using the following expression:

$$\ln P_v = - (4.4 + \ln T_B)$$
$$[1.803(\frac{T_B}{T} - 1)] - 0.803 \ln \frac{T_B}{T} \quad (9)$$
$$- 6.8(\frac{T_M}{T} - 1)$$

where P_v is in torr and T_B, T_M and T are the boiling point, melting point and an environmental temperature (°K), respectively.

Mathematical Model for Soil-Waste Processes—The values developed for degradation and partitioning in the treatability studies for eight pesticides were used as input for the RITZ and VIP mathematical models. The Vadose Zone Interactive Processes (VIP) model is an enhanced version of the Regulatory and Investigative Treatment Zone Model (RITZ). The RITZ model was developed by the EPA, Robert S. Kerr Environmental Research Laboratory, for quantitatively *integrating the processes related to* degradation and transport of organic constituents in the unsaturated zone of a soil system. The VIP model was developed at Utah State University as part of a previous EPA-funded study for use in evaluation of site-specific treatment potential for specific waste-soil mixtures. The major differences between the RITZ and VIP models are the numerical solution algorithms used and the option to use nonequilibrium kinetics in VIP.

Transformation Studies—Transformation studies using radiolabeled 7,12-dimethylbenzanthracene (DMBA) were performed with the McLaurin sandy loam soil at low pH and the same soil adjusted to neutral pH. The distribution of $^{14}CO_2$ between evolved CO_2, soil extracts, and soil residue components was measured to construct a mass balance for DMBA.

Mutagenicity of DMBA and metabolite fractions were measured with the Ames mutagenicity assay. Mutagenic potential of each test smaple was expressed as the mutagenic ratio (MR), i.e., ratio of number of colonies in the presence of a test sample to the number of colonies on a control growth plate in the absence of the test sample.

Results and Discussion

Degradation of PAH Constituents—Results for the Kidman sandy loam (Table 1) generally indicated that PAH persistence increased with increasing molecular weight or compound ring number. The degradation of two-ring PAH compounds, naphthalene and 1 methylnaphthalene, was extensive. Half lives for these PAH compounds were approximately two days. Comparative half lives for the degradation of three-ring PAHs, anthracene and phenanthrene, were 16 and 134 days respectively. Extensive degradation of these two- and three-ring PAH compounds is not unexpected since these compounds can be utilized as a sole source of carbon and energy for soil microorganisms. The four-, five-, and six-

ring PAH compounds were somewhat recalcitrant, exhibiting half lives of greater than 200 days. DMBA, however, was extensively degraded with a half-life of 20 days.

It has been demonstrated that natural soil microorganisms can degrade PAHs by co-metabolic processes. The relative stability of non-substituted high molecular weight PAH compounds in this study suggests that the resident microbial distribution in the soils used may not have included organisms capable of degrading these compounds or a suitable substrate was not present to stimulate co-metabolic decomposition.

These results are consistent with results of other studies using complex wastes. However, higher molecular weight PAH compounds were observed in this study to be more resistant to degradation when present as pure compounds in soil than when present at the same concentrations in the same soil in complex waste mixtures.

Degradation of Pesticides—Toxaphene waste residue exhibited no measurable degradation after 150 days of incubation at an initial soil concentration of 20 mg/kg. The major mechanism for the degradation of toxaphene in soils occurs by reductive dechlorination. Fresh manure was applied to the soil waste mixture (2 percent manure, dry weight basis) to lower redox potential of the soil. Application of manure was not effective in stimulating degradation of toxaphene residue after the same period of incubation. Toxaphene would be classified as persistent in these soils.

Degradation information for pesticides obtained in laboratory treatability studies using the Kidman soil is presented in Table 2. Microbiological degradation of chlorinated pesticides has been reported to follow first-order kinetics. The first-order fit of data generated in this study for many of the chlorinated pesticides was not as good as would be expected if the apparent loss truly followed first-order kinetics. Degradation of organophosphorus pesticides could not be clearly characterized using a first-order reaction kinetic model. Use of first-order kinetics overestimated half-lives for these pesticides.

Chlorinated Hydrocarbons and Aniline—Volatilization corrected degradation rates were determined for the six most volatile chlorinated hydrocarbons in the McLaurin soil (Table 3). Volatilization, as measured by cumulative mass of compound collected on Tenax over the

course of the experiments, was a significant loss mechanism for all compounds studied, ranging from 17 percent for 1,1,2,2-Tetrachloroethane, to over 76 percent for 1,1,2-Trichloroethane.

Partition coefficients—SAR-derived partition coefficients for both experimental soils for chemicals in the four classes evaluated are summarized in Tables 4-6. As expected, PAH and pesticides compound exhibited high K_o and K_d values, while the volatile class of compounds showed high K_h values. Partition coefficients estimated using SARs were in good agreement with literature coefficient values for the compounds addressed.

Model applications—The RITZ and VIP models were used to simulate the behavior of eight pesticides in Kidman soil at a time period beyond the laboratory determined half-life. The organophosphorus pesticides were predicted to degrade significantly in 91 days (96.2 percent for disulfoton to 78.8 percent for parathion). Approximately 70 percent of the applied chlorinated pesticides were predicted to degrade in this time period.

When degradation was eliminated as an input parameter to the models, treatment was limited to the sorptive capacity of the soil for each pesticide. Under these test conditions, transport through volatilization or leaching from the zone of incorporation (ZOI) was not predicted by the models with the exception of toxaphene. Detectable concentrations of toxaphene were predicted to be both volatilized and leached from the zone of incorporation in 91 days.

^{14}C *DMBA results*—Parent ^{14}C DMBA was extensively biodegraded with a half-

Table 1. *Volatilization Corrected Degradation Kinetic Information for PAH Compounds Applied to Kidman Sandy Loam at -0.33 Bar Soil Moisture*

Compound	n	C_o (mg/kg)	k (day^{-1})	$t_{1/2}$ (days)	r^2	95% Confidence Interval			
						Lower Limit		Upper Limit	
						k (day^{-1})	$t_{1/2}$ (days)	k (day^{-1})	$t_{1/2}$ (days)
Naphthalene	12	101	-0.3370	2.1	0.883	-0.4190	1.7	-0.2550	2.7
1-Methylnaphthalene	12	102	-0.4150	1.7	0.922	-0.4960	1.4	-0.3350	2.1
Anthracene	15	210	-0.0052	134	0.829	-0.0065	106	-0.0038	182
Phenanthrene	12	902	-0.0447	16	0.952	-0.0514	13	-0.0380	18
Fluoranthene	15	883	-0.0018	377	0.724	-0.0025	277	-0.0012	578
Pyrene	15	686	-0.0027	260	0.708	-0.0036	193	-0.0017	408
Chrysene	15	100	-0.0019	371	0.804	-0.0024	289	-0.0013	533
Benz(a)anthracene	15	107	-0.0026	261	0.855	-0.0033	210	-0.0020	347
7,12-Dimethylbenz(a)anthracene	12	18	-0.0339	20	0.944	-0.0394	18	-0.0284	24
Benzo(b)fluoranthene	15	39	-0.0024	294	0.830	-0.0030	231	-0.0018	385
Benzo(a)pyrene	15	33	-0.0022	309	0.769	-0.0029	239	-0.0015	462
Dibenz(a,h)anthracene	15	12	-0.0019	361	0.726	-0.0026	267	-0.0013	533
Dibenzo(a,i)pyrene	15	11	-0.0019	371	0.746	-0.0025	277	-0.0013	533
Indeno(1,2,3-cd)pyrene	15	8	-0.0024	288	0.793	-0.0031	224	-0.0017	408

Table 2. *Apparent Loss Kinetic Information for Pesticides from Kidman Soil*

Pesticide	n	C_o (mg/kg)	k (day^{-1})	$t_{1/2}$ (days)	r^2	95% Confidence Interval			
						Lower Limit		Upper Limit	
						k (day^{-1})	$t_{1/2}$ (days)	k (day^{-1})	$t_{1/2}$ (days)
Pentachloronitrobenzene	18	0.300	-0.0398	17	0.925	-0.046	15	-0.034	21
Disulfoton	18	1.56	-0.036	19	0.589	-0.052	13	-0.02	35
Methylparathion	18	1.04	-0.025	28	0.472	-0.039	18	-0.011	63
Phorate	17	1.42	-0.022	32	0.435	-0.036	19	-0.0082	85
Parathion	18	1.45	-0.017	41	0.690	-0.023	30	-0.011	63
Endosulfan	18	0.580	-0.016	43	0.854	-0.02	35	-0.013	53
Aldrin	18	0.429	-0.013	53	0.889	-0.016	43	-0.011	63
Famphur	22	82.7	-0.013	53	0.860	-0.015	46	-0.01	69
Heptachlor	18	0.588	-0.012	58	0.908	-0.014	50	-0.010	70
DDT	18	0.574	-0.015	60	0.524	-0.0173	40	-0.0057	122
Lindane	15	0.394	-0.0113	61	0.384	-0.0199	35	-0.0027	257
Pronamide	17	85.3	-0.0072	96	0.876	-0.0086	81	-0.0057	122
Dinoseb	17	103.1	-0.0067	103	0.890	-0.008	87	-0.0054	128
Aldicarb	22	99.1	-0.0018	385	0.435	-0.0027	257	-0.0008	845
Warfarin	22	117.8	--[a]	--	0.520	--	--	--	--

[a]*Slope (k) of first order regression line is not significantly different from zero, no degradation observed.*

Table 3. Volatilization Corrected Degradation Kinetic Information for Chlorinated Compounds Applied to McLaurin Sandy Loam at -0.33 BAR Coil Moisture Content

| | | | | | | 95% Confidence Interval | | | |
| | | | | | | Lower Limit | | Upper Limit | |
Compound	n	C_0 (mg/kg)	k (day^{-1})	$t_{1/2}$ (days)	r^2	k (day^{-1})	$t_{1/2}$ (days)	k (day^{-1})	$t_{1/2}$ (days)
Degradation Data Corrected for Volatilization, Unpoisoned Soil									
1,1-Dichloroethylene	4	156.0	-16.34	0.04	0.788	-42.14	0.02	--[a]	--
1,1,1-Trichloroethane	4	155.2	-9.60	0.07	0.936	-17.21	0.04	-1.97	0.35
1,1,2-Trichloroethane	6	155	-30.55	0.02	0.599	-65.28	0.01	--	--
1,1,2,2-Tetrachloroethane	6	147	-53.42	0.01	0.588	-115.54	0.01	--	--
Degradation Data Corrected for Volatilization, HgCl Poisoned Soil									
Chloromethylmethyl ether	5	123.6	-55.68	0.01	0.558	-146.69	0.00	--	--
1,1,2-Trichloroethane	5	155	-63.48	0.02	0.536	-172.10	0.00	--	--
1,2-Dibromo-3-chloro-propane	6	144.9	-70.34	0.01	0.516	-164.05	0.00	--	--

[a]Slope (k) of first order regression line is positive, no degradation observed.

Table 4. Calculated Soil/Water (K_d), Oil/Water (K_o), and Air/Water (K_h) Partition Coefficients for PAH Compounds

Compound	Log K_d (McLaurin)	Log K_d (Kidman)	Log K_o	Log K_h
Acenaphthylene	1.72	1.38	4.23	-1.22
Benz(a)anthracene	3.24	2.90	5.95	-5.36
Benzo(a)pyrene	3.67	3.33	6.43	-2.75
Chrysene	3.24	2.90	5.95	-2.41
Dibenzo(a,h)anthracene	3.60	3.26	6.35	-5.52
Ideno(1,2,3-cd)pyrene	5.27	4.93	8.24	-7.62
3-Methylcholanthrene	4.73	4.38	7.63	--
Fluoranthene	2.97	2.62	5.64	-3.60
1-Methylnaphthalene	1.52	1.18	4.00	--
Naphthalene	1.01	0.67	3.42	-1.97
Phenanthrene	2.11	1.76	4.66	-2.30
Pyrene	2.96	2.61	5.63	-4.27
Benzo(b)fluoranthene	4.19	3.86	7.02	-2.91
7,12-Dimethylbenz(a)anthracene	3.61	3.27	6.36	--
Anthracene	2.10	1.75	4.65	-1.59

life of 17 days. Half-life was determined from the decrease of the DMBA ^{14}C fraction over time, which was corrected for abiotic loss and volatilization. These results are consistent with results obtained for a non-radiolabeled DMBA degradation study, which gave biodegradation half-lives of lives of 20 to 28 days. Abiotic loss of ^{14}C DMBA from soil samples poisoned by 2% $HgCl_2$ was statistically not significant (p=0.05). ^{14}C DMBA volatilization was not detected during the 28-day soil incubation period.

The decrease in the parent PAH ^{14}C was accompanied by an increase in metabolite ^{14}C fraction (Table 7). Incorporation of ^{14}C DMBA into a nonextractable soil residue ^{14}C increased from 12 to 17%, however, the increase was not statistically significant (p=0.05). Evolution of ^{14}CO$_2$ was not detected during the 28 days of incubation. These results do not demonstrate that the parent compound was not metabolized to CO_2 since ^{14}C DMBA used was radiolabeled only at the 12 position carbon. In order to detect ^{14}CO$_2$, the benzene ring which contained the carbon-12 was required to be mineralized to CO_2.

Several metabolic intermediate products of DMBA biodegradation were characterized by GC/MS analysis. These included 10-hydroxy-, 4-hydroxy-, and 5-hydroxy-DMBA, respectively. HPLC retention time of these metabolites were identical with those given by reference standards. HPLC elution profile from incubation of ^{14}C DMBA revealed a complex mixture of metabolic products. The elution profile further showed formation of highly polar metabolic products eluting prior to HPLC retention time of DMBA.

Results from Ames assay testing for DMBA metabolites indicated that the highly polar metabolic fraction was mutagenically inactive suggesting that these metabolites may be the detoxified conjugation products of soil microbial enzymes. Moderate and nonpolar metabolite fractions induced a positive response. The mutagenic potential of these metabolite fractions, however, decreased with an increase in soil incubation time. This detoxication potential of DMBA may be important for engineering management and control of hazardous wastes containing this PAH compound since toxicity reduction as a function of incubation time in soil can be used to assess the success of treatment.

Table 5. Calculated Soil/Water (K_d), Oil/Water (K_o), and Air/Water (K_h) Partition Coefficients for 22 Pesticides

Compound	Log K_d (McLaurin)	Log K_d (Kidman)	Log K_o	Log K_h
Aldrin	0.65	0.31	0.62	-1.93
Cacodylic Acid	-2.31	-2.65	-0.32	--
Chlordane, technical	0.44	0.10	2.79	-2.40
DDT	1.14	0.79	3.57	-2.44
Dieldrin	0.56	0.22	2.92	-4.69
Dinoseb	--	--	2.25	--
Disulfoton	-2.31	-2.65	-0.32	-4.13
Endosulfan	1.21	0.86	3.65	-2.44
Heptachlor	1.55	1.21	4.04	-0.97
Alpha Lindane	1.46	1.12	3.94	-4.47
Methyl parathion	0.65	0.31	3.02	-5.56
Parathion	1.06	0.72	3.48	-4.04
Phorate	0.58	0.24	2.94	-3.40
Toxaphene	0.96	0.62	3.37	-5.13
Warfarin	0.19	-0.15	2.49	--
Aldicarb	-1.61	-1.95	0.46	-6.59

Table 6. Calculated Soil/Water (K_d), Oil/Water (K_o), and Air/Water (K_h) Partition Coefficients for Chlorinated Hydrocarbons and Miscellaneous Compounds

Compound	Log K_d (McLaurin)	Log K_d (Kidman)	Log K_o	Log K_h
Chlorinated Hydrocarbons				
Bis-(chloromethyl)ether	-2.68	-3.02	-0.75	--
Chloromethylmethyl ether	-1.41	-1.75	0.69	--
1,2-Dibromo-3-chloropropane Dichlorodifluoromethane	-0.17	-0.51	2.09	2.01
1,1-Dichloroethylene 1,1,1-Trichloroethane	0.13	0.47	2.14	-0.79
1,1,2,2-Tetrachloroethane	2.63	2.29	5.26	-1.81
1,1,2-Trichloroethane	-0.16	-0.50	2.10	-1.51
1,2,2-Trichlorotrifluoroethane	-0.66	-1.01	1.53	--
Hexachlorocyclopentadiene	2.68	2.34	5.31	-1.37
4,4-Methylene-bis-(2-chloroaniline)	0.96	0.62	3.37	--
1,2,4-Trichlorobenzene	1.63	1.29	4.13	-0.77
Miscellaneous Compounds				
Aniline	1.44	1.09	2.34	--
Mitomycin C	8.95	8.61	2.34	--
Pyridine	1.04	0.70	2.13	--
Tetraethyllead	2.28	1.94	2.79	--
Uracil mustard	4.82	4.47	4.13	--

Conclusions

The importance of volatilization and abiotic-loss processes in influencing "apparent loss rates" of substances from soil systems depends upon the class of substances. These processes are insignificant for the majority of PAH compounds. Biodegradation appears to be the major process for loss of PAHs from soil systems. Abiotic loss may be an important process for certain pesticides. Volatilization appears to be the major process influencing loss rates of volatile substances from soil systems.

Transformation products of mutagenic parent substances may exhibit mutagenic characteristics, but may decrease in mutagenic potential with incubation time in soil. A decrease in the concentration of parent substance in a soil extract solution that is not accompanied by an increase in carbon dioxide evolution may not indicate irreversible soil incorporation of applied waste. Rather, intermediate biochemical transformation products may occur that exhibit changing characteristics with time of incubation in the soil.

Mercuric chloride is effective for reducing soil bacteria and fungi to levels at least as low as 10 organisms per gram of soil (dry-weight basis). However, the use of $HgCl_2$ may greatly affect the recovery of certain compounds from soil. The use of $HgCl_2$ sterile controls for biodegradation studies should be further examined.

It is possible to develop transport information for mathematical models by calculating partition coefficients based on structure-activity relationships for substances that are difficult to evaluate experimentally.

Under environmental and loading rate conditions representative of well designed and well managed soil treatment systems, very little leaching or air emissions of either pesticides or PAH compounds was predicted by the RITZ or VIP models using soil fate and transport input data generated in laboratory experiments or in literature citations.

Table 7. Transformations of (^{14}C) 7,12-Dimethylbenz(a)anthracene by McLaurin Sandy Loam Soil[a]

Time (days)	^{14}C appearing in each fraction (%)				
	Soil Extract				
	7,12-Dimethylbenz(a)-anthracene (parent compound)	Metabolites	Soil Residue	CO_2	Total
0	62 (69)	4 (6)	12 (13)	0 (0)	78 (88)
14	26	43	16	0	85
28	20 (60)	53 (11)	17 (16)	0 (0)	90 (87)

[a]Poisoned (control) data in parentheses.

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