Proceedings of the 1988 Winter Simulation Conference
M. Abrams, P. Haigh, and J. Comfort (eds.)

Comparison of an unsaturated soil zone model (SESOIL) predictions with a laboratory leaching experiment

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ABSTRACT

Model predictions of a modified version of the soil compartment model SESOIL are compared with laboratory measurements of pollutant transport in soil. A brief description of SESOIL is given and modifications that have been made to the model are summarized. Comparisons are performed using data from a laboratory soil column study involving six chemicals (dicamba, 2,4-dichlorophenoxyacetic acid, atrazine, diazinon, pentachlorophenol, and lindane). Overall, SESOIL model predictions are in good agreement with the empirical data. Limitations of the model are discussed.

INTRODUCTION

The SEasonal SOIL model SESOIL (Bonazountas and Wagner, 1984), a code developed for the U. S. Environmental Protection Agency (EPA) Office of Toxic Substances (OTS), estimates concentrations of pollutants in the soil following introduction via direct application and/or interaction with other media (i.e., deposition from air). The soil hydrology submodel of SESOIL has been evaluated by Hetrick et al. (1984, 1986) and a number of other studies have been conducted on the SESOIL model including sensitivity analysis, comparison with other models, and some limited comparisons with measured data (Bonazountas et al., 1982; Wagner et al., 1983; Kincaid et al., 1984; Melancon et al., 1986; Watson and Brown, 1985). The purpose of this paper is to present a study of the performance of the pollutant transport cycle submodel of an improved version of SESOIL. The comprehensive evaluation of SESOIL performed by Watson and Brown (1985) uncovered numerous deficiencies in the model, and thus the SESOIL code has been extensively modified at Oak Ridge National Laboratory (ORNL) to enhance its capabilities.

We have evaluated the performance of the modified SESOIL by comparing its predictions to published experimental data for pollutant transport in the soil column from a laboratory study by Melancon et al. (1986) involving six organic chemicals (dicamba, 2,4-dichlorophenoxyacetic acid, atrazine, diazinon, pentachlorophenol, and lindane). Unknown hydrologic parameters were calibrated until components of the hydrologic cycle of the model compared well with limited measurements; predictions of components of the pollutant cycle were then compared to available data. Results from both the new and old versions of SESOIL will be given. Conclusions regarding SESOIL's performance and limitations are presented.

SESOIL is incorporated into EPA's Graphical Exposure Modeling System (GEMS), a system developed to support integrated exposure analysis at OTS (Kinerson and Hall, 1986). The model is maintained by OTS of EPA; interested users should contact R. S. Kinerson, OTS, Washington, D. C..

SESOIL MODEL DESCRIPTION

The SESOIL model (Bonazountas and Wagner, 1984) estimates pollutant concentrations in the soil profile following introduction via direct application and/or interaction with other media (i.e., deposition from air). The model defines the soil compartment as a soil column extending from the ground surface through the unsaturated zone and to the upper level of the saturated soil zone. Processes simulated in SESOIL are categorized in three cycles - the hydrologic cycle, sediment cycle, and pollutant cycle. Each of the three cycles are separate submodels in the SESOIL code. The hydrologic cycle includes rainfall, surface runoff, infiltration, soil water content, evapotranspiration, and groundwater runoff. The sediment cycle includes soil erosion which occurs due to surface runoff. The pollutant cycle includes convective transport, volatilization, adsorption/desorption, and degradation/decay. The SESOIL model does not address pollutant movement in saturated groundwater.

Watson and Brown (1985) tested and evaluated the SESOIL model and found numerous deficiencies. The code has subsequently been extensively modified. The modifications have been reported by Hetrick et al. (1988) and are now summarized. The new SESOIL includes a chemical-specific retardation factor whereas before all chemicals would reach the groundwater at the same time, irrespective of their chemical sorption characteristics. For better resolution, the model was discretized so that each of up to four major soil layers can have up to ten sublayers, each having the same soil properties as the major layer in which they reside. The volatilization algorithm was modified so that if the chemical is in the second or lower layer, and the concentration in that layer is greater than the layer above it, then the chemical will diffuse into the upper layer rather than volatilize directly into the atmosphere as before. A pure chemical phase was added to the model so that the simulated pollutant concentration in the dissolved (soil water) phase can not exceed the solubility of the chemical. The model was modified to predict soil temperature from air temperature rather than assume that soil temperature is equal to air temperature as before. A new option was added to the input capabilities of SESOIL that allows a spill loading. Other miscellaneous modifications were made including rewriting the subroutine that prints results to be more efficient and so that the output would be more readable.

SESOIL is considered to be a screening-level model and thus data requirements are not extensive, utilizing a minimum of soil and chemical parameters and monthly or seasonal meteorological values as input. Output of the SESOIL model includes pollutant concentrations at various soil depths and pollutant loss from the unsaturated soil zone in terms of surface runoff, percolation to groundwater, volatilization, and degradation. Complete descriptions of the SESOIL algorithms can be found in Bonazountas and Wagner (1984). The three major cycles are summarized by Hetrick et al. (1988).

VALIDATION DESIGN

The modified SESOIL was evaluated by comparing its predictions with published experimental data. These include transit time through the soil column, the amount of pollutant in daily effluent samples, the time-dependent depth distribution of the pollutant, and the mass balance at any time (cumulative mass in soil, in leachate, and in the degradation and volatilization components.) The sum of the mass balance components should equal the amount of chemical applied initially. The data used in this evaluation are now summarized.

Melancon et al. (1986) filled four two-meter columns (59.4 cm inside diameter) with sandy soil, applied a chemical to the surface, and watered each column for 30 days. A total of 285 cm water was added to each column during that time. This is roughly an order of magnitude higher infiltration than normally expected from rainfall. The quantity of chemical leachate was recorded on a daily basis. After the 30 days the experiment was stopped; each soil column was broken down and the amount of pollutant remaining in every five centimeter section of the column was measured. Six organic chemicals were studied: 2,4-dicloro-phenoxyacetic acid (2,4-D), atrazine, diazinon, dicamba, lindane, and pentachlorophenol (PCP). The values for sorption, degradation rate, and the Freundlich exponent were determined in the laboratory (Lopez-Avila et al., 1985a, 1985b). These chemicals cover a wide range of adsorption coefficients (see Table 1) and thus constitute a reasonably thorough test of any modeling program.

Melancon et al. (1986) compared the results of their soil column studies to the predictions of three soil modeling programs: PESTAN (Enfield et al., 1982), PRZM (Carsel et al., 1984), and the old version of SESOIL (Bonazountas and Wagner, 1984). The values Melancon et al. measured for various model input parameters, such as the degradation rate and the adsorption coefficient, differed markedly from values published in the literature. Frequently, users of transport models are forced to use data from some published source (based upon general soil type) since little site-specific information is available. Therefore, Melancon et al. (1986) ran each model twice, once with input parameters obtained from the literature and once with their measured input parameters, to see how the differences affected the results.

For this study, the input parameters were obtained from Melancon et al. (1986) and tested first with the old version of SESOIL to verify their results. Testing then began on the new SESOIL version. Note that daily leachate results are not provided by SESOIL. Thus the old version of SESOIL was not tested in this regard. The new code was temporarily modified to print out the daily leachate so that these results could be compared to the experimental data along with the end-of-the-month distribution data. Both the measured and the literature input parameters were used (see Table 1).

In order to make the hydrology of the model agree more closely with the experimental setup, the values of K1 (the soil intrinsic permeability) and c (the soil disconnectedness index) were varied to reduce the predicted surface runoff to below 1 cm per month while maintaining the predicted soil water content at about the measured value (approximately 0.125 cm^3/cm^3). This procedure is recommended in the SESOIL user's guide (Bonazountas and Wagner, 1984) and is discussed by Hetrick et al. (1986) in their study of the SESOIL hydrologic cycle. The parameter c is defined as the exponent relating the "wetting" or "drying" time-dependent permeability of a soil to its saturated permeability (Eagleson, 1978), and typically ranges in value from 12 for clay type soils to 3.7 for sandy soils. The same values of K1 and c were used in both the measured and the literature runs.

Table 1. Summary of Rate Constants and Other Model Input Data Used in SESOIL Based on Literature Values and Laboratory Measurements (Melancon et al., 1986)

	Dicamba	2,4-D	Atrazine	Diazinon	PCP	Lindane
Adsorption Coefficient K_d (cm^3/g)						
Literature	0.002	0.021	0.168	0.678	0.945	2.625
Measured	0.120	0.140	0.493	1.632	3.341	3.530
Solubility (mg/l)[a]	4500	900	33	40	14	7.8
Degradation Rate (d^{-1})						
Literature	0.065	0.040	0.010	0.015	0.033	0.005
Measured	0.009	0.140	0.009	0.032	0.025	0.032
Freundlich Exponent						
Literature	0.850	1.330	1.140	1.000	2.380	1.020
Measured	1.120	0.960	1.360	1.110	1.210	1.230
Henry's Law Constant[a]	1.29E-9	1.939E-10	7.29E-9	1.40E-6	2.80E-6	7.80E-6
Neutral Hydrolysis Rate Constant[a]	0	0	0	4.30E-8	0	0
Acid Hydrolysis Rate Constant[a]	0	0	0	2.10E-2	0	0
Basic Hydrolysis Rate Constant[a]	0	0	0	5.30E-3	0	0
Molecular Weight	221.04	221.04	216.06	304.36	266.35	290.85
Diffusion Coefficient in Air (cm^2/s)[a]	6.05E-2	6.05E-2	5.93E-2	5.54E-2	5.92E-2	5.58E-2

Soil Parameters	Bulk Density (g/cm^3)	Porosity (cm^3/cm^3)	Organic Carbon (%)	Intrinsic Perm. (cm^2)	Disconn. Index c
Literature	1.57	0.35	a	1.1E-7	4.6
Measured	1.38	a	.105	a	a

Environmental Parameters	Temp. (°C)	Relative Humid. (%)	Evap. (cm/d)	Albedo (-)	Watering Rate (cm/d)	Cloud Cover (frac)
Literature	29.6	42.0	1.13	0.250	9.67	0.32
Measured	26.7	66.7	.189	0.220	9.67	0.32

[a] Same values used for both literature and measured runs.

RESULTS AND DISCUSSION

Results from the modified SESOIL model agreed more closely with the experimental data than the old SESOIL version (see Melancon et al., 1986). The new chemical retardation factor used in SESOIL to control chemical movement in the soil produces adequate results as can be seen in Table 2. The breakthrough days (days in which the chemicals appeared at bottom of soil column) predicted by SESOIL using the measured input parameters were generally quite close to the actual breakthrough days (see Table 2); at worst there was a difference of five days. The previous version of SESOIL predicted that all six chemicals appeared at the bottom of the soil column during the third day. The advantage of using the measured input parameters rather than those from the literature is quite apparent. The best prediction using literature values disagrees by three days; the worst disagrees by 14 days. In all cases the results of SESOIL predicted that the pollutant would reach the bottom of the soil column faster than the measurements showed.

SESOIL's predictions of the mass balance after 30 days using both the measured and literature data for input are compared to the experimental measurements in Table 3. Results from the PESTAN, PRZM, and old SESOIL models are given also (Melancon et al., 1986). All SESOIL (new version) predicted values from runs with the measured input parameters except those for atrazine are within a factor of two of the experimental values. As can be seen in Table 3, the old version of SESOIL did not do this well. All four models predicted the bulk of the chemical atrazine would leach through the columns more quickly than was actually observed in the experiments.

SESOIL model predictions using measured input parameters versus literature-derived input parameters compared better to the experimental data for 2,4-D, atrazine, and diazinon. However, model predictions using the measured values did not improve for PCP and lindane, the two chemicals with the highest adsorption coefficients, or for dicamba which had the lowest adsorption coefficient of the chemicals studied. Results from the PRZM model were very similar to those from SESOIL for these three chemicals.

SESOIL results for the total chemical concentration in soil versus depth (at the end of 30 days) are compared graphically to observations from the four soil columns in Figure 1, while the predicted distributions of the amount of pollutant in the leachate versus time are compared to the measurements in Figure 2. Note that atrazine was the only chemical that was found in both leachate and soil samples in the laboratory study. The darkened lines in the figures show SESOIL results using measured input data, the dashed lines show results using literature input

Table 2. Day of Chemical Breakthrough in Effluent Samples and SESOIL Results

	Breakthrough Days
2,4-D	
Measured:	10, 12, 11, 11 (4 soil columns)
SESOIL Results:	
Measured Input Data:	7
Literature Input Data:	4
Atrazine	
Measured:	21, 21, 23, 23
SESOIL Results:	
Measured Input Data:	18
Literature Input Data:	9
Dicamba	
Measured:	6, 7, 7, 7
SESOIL Results:	
Measured Input Data:	7
Literature Input Data:	3
Diazinon	
Measured:	>30 days
SESOIL Results:	
Measured Input Data:	>30 days
Literature Input Data:	27

Measurements nor SESOIL results "broke through" the columns within 30 days for Lindane or PCP.

Table 3. Mass Balance Calculations for Measured Chemical Data (Average from 4 Columns) vs. PESTAN, PRZM, Old SESOIL, and New SESOIL Model Predictions, Showing Cumulative Mass (mg) in Soil, Leachate, and Degradation Components on Day 30 (Based on 250.5 mg Initial Loading). Numbers in Parentheses Show 95% Confidence Limits About the Average Measured Data (p=0.05).

	Literature Runs			Measured Runs		
	Soil	Leachate	Degradation	Soil	Leachate	Degradation
Dicamba						
PESTAN	-	22.0	228.4	-	169.6	80.5
PRZM	-	214.9	35.6	-	233.9	16.5
Old SESOIL	21.6	190.0	38.9	56.0	189.0	5.2
New SESOIL	-	199.9	50.6	.0009	234.0	16.5
Meas.	-	216.7(±96.6)	33.8[a]	-	216.7(±96.6)	33.8[a]
2,4-D						
PESTAN	-	82.8	167.8	-	4.3	246.3
PRZM	-	221.0	29.4	-	81.5	168.9
Old SESOIL	30.1	196.0	24.4	45.1	138.0	66.7
New SESOIL	.0003	210.8	39.7	-	80.9	169.6
Meas.	-	48.7(±24.1)	201.8[a]	-	48.7(±24.1)	201.8[a]
Atrazine						
PESTAN	-	242.4	8.1	2.0	189.5	58.9
PRZM	-	231.3	29.1	4.8	210.0	35.5
Old SESOIL	80.1	165.0	5.4	164.6	82.4	3.4
New SESOIL	.057	226.2	24.3	24.3	183.2	42.9
Meas.	94.8(±22.2)	4.0(±2.6)	151.7[a]	94.8(±22.2)	4.0(±2.6)	151.7[a]
Diazinon						
PESTAN	-	246.5	7.0	152.2	-	98.2
PRZM	4.8	18.7	226.9	96.7	0.9	152.8
Old SESOIL	164.9	65.8	5.2	213.8	13.3	5.6
New SESOIL	87.6	56.6	106.3	86.2	-	164.3
Meas.	47.2(±18.2)	-	203.3[a]	47.2(±18.2)	-	203.3[a]
PCP						
PESTAN	105.0	-	157.4	203.0	-	47.2
PRZM	71.1	29.1	150.2	120.4	-	130.0
Old SESOIL	247.0	0.3	3.6	248.2	0.5	2.0
New SESOIL	98.7	-	151.8	120.3	-	130.2
Meas.	76.2(±38.5)	-	174.3[a]	76.2(±38.5)	-	174.3[a]
Lindane						
PESTAN	238.3	-	13.2	192.6	-	57.4
PRZM	215.6	-	34.8	96.4	-	154.0
Old SESOIL	244.1	4.8	1.2	247.5	0.3	2.3
New SESOIL	185.2	-	65.3	96.2	-	154.3
Meas.	179.6(±25.4)	-	70.9[a]	179.6(±25.4)	-	70.9[a]

[a] Chemical unaccounted for in either the observed effluent or soil samples is assumed lost to degradation.

values, and the light lines are the measurements from the four soil columns. There was a trend for SESOIL to more closely approximate observed chemical peak location, height, and distribution when measured rate information rather than literature-derived values were used. This was not the case before when using the previous SESOIL version that allowed only four layers between the surface and groundwater. The predictions using the old SESOIL code did not improve with the use of measured rate constant information (see Melancon et al., 1986). This study shows the importance of discretizing the SESOIL model to become essentially a n-layered model and the effect of using a chemical retardation factor.

CONCLUSIONS

Predictions of the improved version of the model code SESOIL were compared to empirical data from a laboratory study involving six organic chemicals. Results for several aspects of pollutant transport were compared including the time-dependent amount leached through the bottom of the soil column, the depth distribution of the pollutant at various times, and the mass of the chemical degraded.

Overall, SESOIL model predictions are in good agreement with observed data. The modified SESOIL does a better job of predicting the leading edge of the chemical

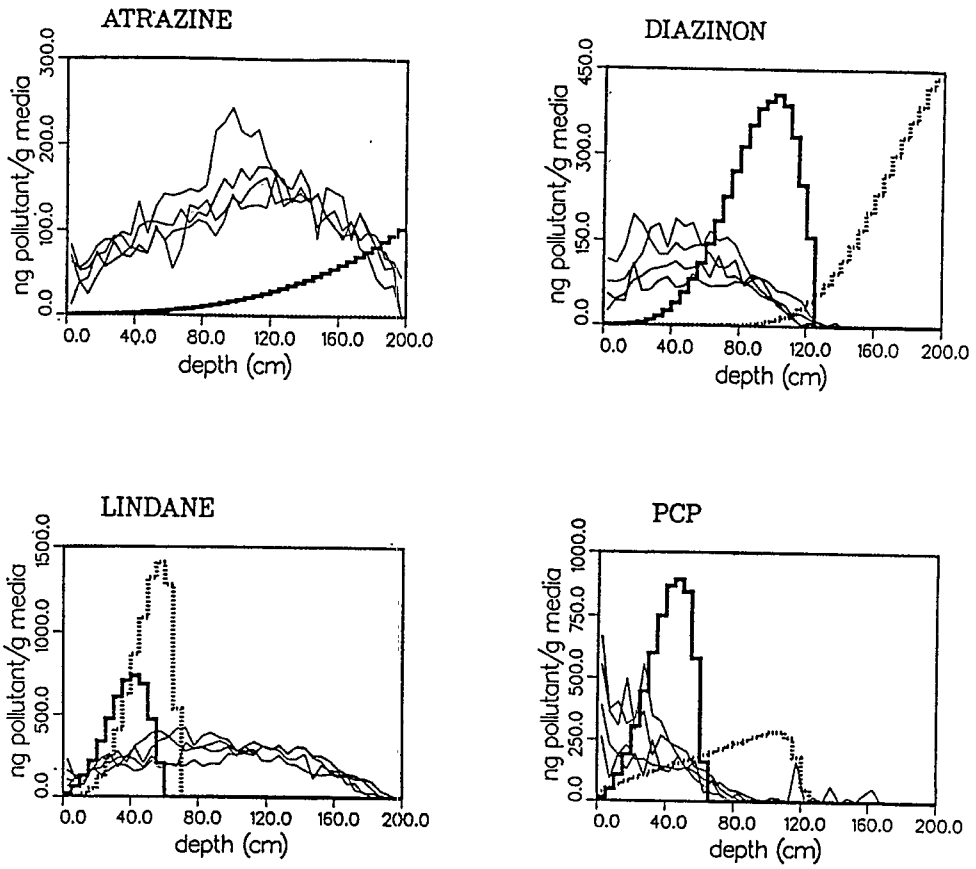

Figure 1: Results of SESOIL "Measured" (dark line) and "Literature" (dashed line) simulations compared with column data (light lines) for atrazine, diazinon, lindane, and PCP.

profile than the old SESOIL due mainly to improving the pollutant penetration algorithm to include the chemical sorption characteristics. Mass balance calculations by the new SESOIL code were improved over the old version, especially when measured input parameters rather than those from the literature were used.

It is felt that SESOIL can be a useful screening-level chemical migration and fate model. The model is relatively easy to use, input data are straightforward to compile, and most of the model parameters can be obtained or readily estimated. SESOIL can be applied to generic environmental scenarios for purposes of evaluating the general behavior of chemicals. SESOIL should not be applied on a site-specific basis with only limited calibration. Caution should be used when making conclusions based on modeling results when little data exist against which to calibrate predictions. However, the simulations in this paper do indicate that SESOIL, when properly used, can be an effective screening-level tool in assessing chemical movement in soils.

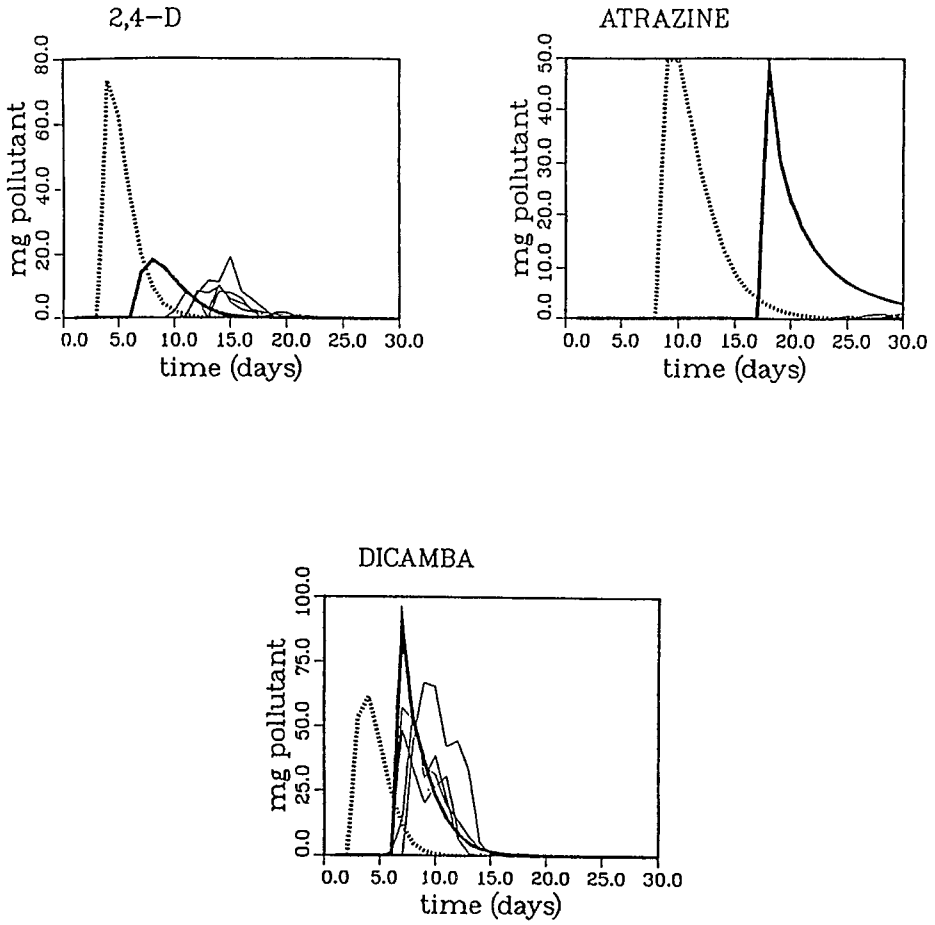

Figure 2: Results of SESOIL "Measured" (dark line) and "Literature" (dashed line) simulations compared with column data (light lines) for 2,4-D, atrazine, and dicamba.

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