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LATIN HYPERCUBE SAMPLING WITH THE SESOIL MODEL

David M. Hetrick, Robert J. Luxmoore,* and M. Lynn Tharp
Computing Applications Division
Oak Ridge National Laboratory+
Oak Ridge, Tennessee 37831

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Latin Hypercube Sampling With The SESOIL Model

David M. Hetrick, Robert J. Luxmoore, and M. Lynn Tharp
Oak Ridge National Laboratory
P.O. Box 2008, M.S. 6180
Oak Ridge, TN 37831
(615) 576-7556

I. ABSTRACT

The seasonal soil compartment model SESOIL,[1,2] a one-dimensional vertical transport code for chemicals in the unsaturated soil zone, has been coupled with the Monte Carlo computer code PRISM,[3] which utilizes a Latin hypercube sampling method. Frequency distributions are assigned to each of 64 soil, chemical, and climate input variables for the SESOIL model, and these distributions are randomly sampled to generate N (200, for example) input data sets. The SESOIL model is run by PRISM for each set of input values, and the combined set of model variables and predictions are evaluated statistically by PRISM to summarize the relative influence of input variables on model results. Output frequency distributions for selected SESOIL components are produced.

As an initial analysis and to illustrate the PRISM/SESOIL approach, input data were compiled for the model for three sites at different regions of the country (Oak Ridge, Tenn.; Fresno, Calif.; Fargo, N.D.). The chemical chosen for the analysis was trichloroethylene (TCE), which was initially loaded in the soil column at a 60- to 90-cm depth. The soil type at each site was assumed to be identical to the cherty silt loam at Oak Ridge; the only difference in the three data sets was the climatic data. Output distributions for TCE mass flux volatilized, TCE mass flux to groundwater, and residual TCE concentration in the lowest soil layer are vastly different for the three sites.

II. INTRODUCTION

Computer simulation models for the fate and transport of chemicals in soils are being used for guidance in identifying residual chemical concentrations in the soil column which will have little or no affect on groundwater quality. Different regions of the United States can be expected to have different levels of acceptable soil contamination because of the wide range of soils, vegetation, and climatic conditions. An initial simulation investigation has been completed that demonstrates the different soil cleanup criteria required for different regions of the United States.

The screening-level code SESOIL, a one-dimensional vertical transport and fate model for chemicals in the unsaturated soil zone, was selected for this work based on SESOIL's wide use in waste-site assessments. SESOIL was developed at Arthur D. Little, Inc., by Bonazountas and Wagner,[1] and enhanced and modified at Oak Ridge National Laboratory (ORNL) by Hetrick et al.[2] under Environmental Protection Agency (EPA) sponsorship. Following SESOIL's release by EPA, the model has been developed as a component of the RISKPRO^{tm} software by General Sciences Corporation[4] for assessment applications. SESOIL has been applied to soil cleanup levels in California[5,6] and to site sensitivity ranking for Wisconsin soils for the Wisconsin Department of Natural Resources.[7]

An important aspect for determining soil cleanup criteria is the uncertainty that arises due to the variability of soil, vegetation, chemical, and climate factors that control chemical fate and transport. Monte Carlo simulation methods have been used to relate the uncertainties in transport model predictions and variability of model inputs. For this study, the Latin hypercube sampling method was used as a means of propagating frequency distributions through the SESOIL code to obtain frequency distributions of output variables, such as chemical flux to groundwater, volatilization flux, and residual chemical concentration in soil. The purpose of this paper is to illustrate the PRISM/SESOIL approach and to present a preliminary analysis for three sites from different regions of the country.

III. METHOD

The Monte Carlo computer code called PRISM,[3] which uses Latin hypercube sampling, was linked with the seasonal soil compartment model SESOIL,[1,2] a one-dimensional vertical transport code for the unsaturated soil zone. In PRISM (see Fig. 1), frequency distributions for 64 soil, chemical, and climate variables for SESOIL (see Table 1) are divided into N equal-probability classes (200, for example). Note that three precipitation variables, each having monthly values, comprise 36 of the 64 inputs. These distributions are randomly sampled to generate N input data sets. PRISM reads each set of input values, runs the SESOIL model, and outputs the model predictions. PRISM statistically evaluates the joint set of model variables and predictions, and indicates the most sensitive input variables for given output variables. Frequency distributions can be produced for up to eleven output variables that were selected for examination (see Table 2).

Initially, a sensitivity analysis was done to aid in selection of variables that had the most influence on model predictions. For a sensitivity analysis, the coefficient of variation (100 * standard deviation / mean) on each of the 64 parameters is set at 1% (i.e., a normal distribution with the standard deviation set at 1% of the mean). Based on this analysis, 9 of the 64 input variables were selected, and frequency distributions were assigned. Normal distributions were arbitrarily selected for state variables (bulk density, RS; disconnectedness index, C; porosity, N; and organic carbon content, OC) and log-normal distributions assigned for flux variables (air diffusion coefficient, DA and intrinsic permeabilities, K11, K12, K13, and K14 for four soil layers). All other variables that could be assigned frequency distributions in PRISM/SESOIL were held constant at their mean values for this analysis.

Thus, for this study, the nine input distributions were divided into 200 equal probability classes and sampled randomly, without replacement, to generate 200 input data sets (PRISM1 in Fig. 1). These 200 data sets contain random combinations of the variability represented in the input distributions. SESOIL was run 200 times using each of the assembled data sets (PRISM2 in Fig. 1). Finally, the statistical analysis (PRISM3 in Fig. 1) ranks the influence of input variables for each model prediction. The Statistical Analysis System (SAS)[8] was used to calculate the mean, standard deviation, and minimum and maximum values for each output distribution, and to produce the output frequency distributions.

IV. EXAMPLE ANALYSIS

For an initial analysis, input data were compiled for three different sites at different regions of the United States (Oak Ridge, Tenn.; Fresno, Calif.; Fargo, N.D.). The chemical chosen for the analysis was TCE since it is one of the most common pollutants found at Superfund sites and is classified as a probable human carcinogen by EPA. It was assumed that the soil type at each site was identical to the cherty silt loam selected for the Oak Ridge site application. Thus, the only differences in the three input data sets were the climatic data. Long-term monthly average climate data for SESOIL for each site were obtained from the climate database in the RISKPRO[tm] system, an information management tool designed to help users perform exposure assessments.[4]

The soil column was discretized into four soil horizons (60, 90, 150, and 200 cm thicknesses), each having 3 sublayers for a total of 12 sublayers. PRISM/SESOIL was run for each site for 10 years; each run used 200 simulations. In each case an initial loading of 300 μg of TCE was input to the first sublayer of the second soil horizon (60-90-cm depth). The 200 simulations for each site took approximately 8.8 hours to run on an IBM RISC System/6000 workstation.

V. RESULTS

The simulation results presented here are intended to illustrate the approach and should not be taken as predictions. SAS was used to statistically evaluate results for each site for TCE mass volatilized, TCE mass transported to groundwater, and TCE concentration in the lowest soil sublayer (VOLAT#, GRNWTR#, and PCONC4L#, respectively from Table 2) for each of 10 years (# from 1 to 10). Tables 3-5 show results for the mean, standard deviation, minimum, and maximum for each parameter for the Oak Ridge, Tenn.; Fresno, Calif.; and Fargo, N.D. sites, respectively. Note that most of the chemical migrated to the groundwater during years 2 to 6 at the Oak Ridge site, but at the Fresno site most of the TCE volatilized to the atmosphere during the first 5 years. At Fargo, volatilization was the greater flux during the first 4 years, with greater groundwater flux after year 4. The chemical concentration in the lowest soil layer at the end of the 10-year simulation was highest at the Fargo site.

The relative frequency distributions (frequency/number of iterations) for VOLAT, GRNWTR, and PCONC4L for selected years at each site show a range of skewed distributions (see Figs. 2-10). The TCE mass to groundwater for Oak Ridge and Fargo showed a normal distribution in year 2 and year 7, respectively (Figs. 2 and 8), whereas the equivalent distribution for Fresno in year 8 was strongly skewed to the left (Fig. 5). Fresno showed a normal distribution for volatilization flux in year 1 (Fig. 6), while for Oak Ridge and Fargo the distributions for volatilization flux were skewed to the left (Figs. 3 and 9, respectively). The soil concentration distribution was normal for Oak Ridge in year 2 (see Fig. 4), was skewed to the left at Fresno in year 7 (Fig. 7), and was skewed to the right in year 6 at the Fargo site (Fig. 10). While results shown here should be considered preliminary, it is apparent that the three sites have differing rates of TCE transport by volatilization and drainage to groundwater. These results infer that different cleanup guidelines may be appropriate for contrasting sites based on climatic differences.

VI. SUMMARY/DISCUSSION

The search for suitable cleanup criteria for soils can be expected to show that differing levels of soil contamination may be considered benign in different regions of the United States because of differing sensitivities of hydrologic and vapor transport to the wide range of soil, vegetation, and climatic conditions. Computer simulation modeling is being used as a guide to identifying residual concentrations of chemical wastes in soil which have little or no significant effect on groundwater quality. To aid in involving uncertainty analysis with the computer modeling effort, the Monte Carlo computer code, PRISM, which uses Latin hypercube sampling, was linked with the seasonal soil compartment model SESOIL.

The appeal of using SESOIL for this approach is that SESOIL uses less soil, chemical, and meteorological values as input than similar models, while still considering the most important transport and transformation processes. Also, databases are available in RISKPRO™ [4] to facilitate the gathering of data for the model.

The PRISM/SESOIL approach was illustrated by investigating the fate and transport of TCE at three sites in different areas of the United States (Oak Ridge, Tenn.; Fresno, Calif.; and Fargo, N.D.). Simulations have been used to evaluate the uncertainties associated with several input variables for the three sites. The TCE transport and fate varied across the three sites considered, based on regional climatic differences. The implications of region-to-region differences compared with site-to-site differences within a given region are under study, and further PRISM/SESOIL simulations are planned.

VII. ACKNOWLEDGMENTS

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Table 1. SESOIL Input Parameters That Can Have Input Distributions	
RS	average soil bulk density (g/cm^3)
K1	average soil intrinsic permeability (cm^2)
C	soil pore disconnectedness index (-)
N	effective porosity (-)
OC	organic carbon content (%)
CEC	cation exchange capacity (milli eq./100 g dry soil)
FRN	Freundlich equation exponent (-)
DA	air diffusion coefficient (cm^2/s)
KOC	organic carbon adsorption coefficient (μg/g-oc)/(μg/ml)
K	adsorption coefficient (μg/g)/(μg/ml)
KDEL	liquid phase biodegradation rate (day^{-1})
KDES	solid phase biodegradation rate (day^{-1})
D1	thickness of upper-most soil layer (cm)
D2	thickness of second soil layer (cm)
D3	thickness of third soil layer (cm)
D4	thickness of bottom soil layer (cm)
PH1	pH of the upper-most layer (-)
PH2	pH of the second soil layer (-)
PH3	pH of the third soil layer (-)
PH4	pH of the bottom soil layer (-)
K11	intrinsic permeability for the upper-most layer (cm^2)
K12	intrinsic permeability for the second soil layer (cm^2)
K13	intrinsic permeability for the bottom soil layer (cm^2)
K14	intrinsic permeability for the bottom soil layer (cm^2)
MPA#	precipitation for month # where # is 1 to 12 (cm)
MTR#	mean duration of storm events for month # (-)
MN#	mean number of storm events for month # (-)
(MPA#, MTR#, AND MN# are long-term monthly averages for the site)	
RUNL1	initial pollutant loading in upper-most layer ($\mu g/cm^2$)
RUNL2	initial pollutant loading in layer 2 ($\mu g/cm^2$)
RUNL3	initial pollutant loading in bottom layer ($\mu g/cm^2$)
RUNL4	initial pollutant loading in bottom layer ($\mu g/cm^2$)

Table 2. PRISM/SESOIL Model Output Variables

Hydrologic Cycle Parameters:	
THETAU#	average soil water content for year # (%)
INF#	total water infiltration for year # (cm)
EVAP#	total evapotranspiration for year # (cm)
SUR_RUN#	total surface runoff for year # (cm)
GRW_RUN#	total groundwater runoff for year # (cm)
MOI_RET#	total water retention for year # (cm)
Pollutant Cycle Parameters:	
VOLAT#	total pollutant mass flux volatilized for year # (μg/year)
GRNWTR#	total pollutant mass flux to groundwater for year # (μg/year)
PDEG#	total pollutant degraded for year # (μg/year)
PCONC4L#	average pollutant concentration in the lowest layer for year # (μg/ml)
PCONC4L#	average pollutant concentration in the lowest layer for year # (μg/ml)
TMASij#	end-of-year total pollutant mass for layer i, sublayer j, and year # (μg)

Table 3. PRISM/SESOIL Results for Oak Ridge, Tenn.					
Variable	N	Mean	Std Dev	Minimum	Maximum
VOLAT1	200	0.5714642	0.7683233	0.0272233	8.7824600
VOLAT2	200	0.0517445	0.1902608	0.000047337	2.5537000
VOLAT3	200	0.0290044	0.1205273	0.000014291	1.6369200
VOLAT4	200	0.0182598	0.0823770	5.3958E-6	1.1261200
VOLAT5	200	0.0116538	0.0565760	2.08777E-6	0.7772370
VOLAT6	200	0.0074846	0.0388970	8.32818E-7	0.5364640
VOLAT7	200	0.0048334	0.0267587	3.90379E-7	0.3702230
VOLAT8	200	0.0031372	0.0184154	2.52454E-7	0.2554470
VOLAT9	200	0.0020460	0.0126775	2.13086E-7	0.1762270
VOLAT10	200	0.0013405	0.0087307	9.05057E-8	0.1215770
GRNWTR1	200	1.6590964	4.3520087	0	34.8383000
GRNWTR2	200	105.4000245	23.2881755	27.6176000	156.8040000
GRNWTR3	200	81.7097075	4.5919946	66.3128000	93.5881000
GRNWTR4	200	46.5357875	5.0456514	25.6104000	57.6719000
GRNWTR5	200	26.5572110	4.9613132	9.8494900	39.8335000
GRNWTR6	200	15.2647334	4.1052738	3.7875500	27.5102000
GRNWTR7	200	8.8386198	3.1151876	1.4568300	18.9945000
GRNWTR8	200	5.1552620	2.2552937	0.5601270	13.1119000
GRNWTR9	200	3.0290874	1.5896897	0.2154950	9.0488000
GRNWTR10	200	1.7920331	1.1029525	0.0828670	6.2429300
PCONC4L1	200	0.4452984	0.3196424	0	1.6909100
PCONC4L2	200	2.2578174	0.1989653	1.5751300	2.7567000
PCONC4L3	200	1.5139894	0.1257451	1.0875100	1.9197500
PCONC4L4	200	0.8644593	0.1325038	0.4196780	1.2435800
PCONC4L5	200	0.4952767	0.1162779	0.1613890	0.8443570
PCONC4L6	200	0.2858231	0.0912536	0.0620666	0.5731530
PCONC4L7	200	0.1661638	0.0674089	0.0238716	0.3914080
PCONC4L8	200	0.0973112	0.0480968	0.0091791	0.2701780
PCONC4L9	200	0.0574076	0.0336280	0.0035312	0.1864450
PCONC4L10	200	0.0340987	0.0232261	0.0013579	0.1286350

Table 4. PRISM/SESOIL Results for Fesno, Calif.					
Variable	N	Mean	Std Dev	Minimum	Maximum
VOLAT1	200	157.9299145	41.8599112	63.6883000	278.2750000
VOLAT2	200	52.0573440	6.1740980	17.1038000	60.9525000
VOLAT3	200	27.6635698	5.5360850	3.4803600	34.4394000
VOLAT4	200	16.4940083	5.1167690	0.7877740	23.3928000
VOLAT5	200	10.5257723	4.2944928	0.1817650	16.9270000
VOLAT6	200	7.2692735	3.5906399	0.0575110	13.7634000
VOLAT7	200	5.1645771	2.9747952	0.0185911	11.3793000
VOLAT8	200	3.8008059	2.4687841	0.0058808	9.3975800
VOLAT9	200	2.8959156	2.0822121	0.0022654	7.9700400
VOLAT10	200	2.2496710	1.7756109	0.000927951	7.0043500
GRNWTR1	200	0	0	0	0
GRNWTR2	200	0	0	0	0
GRNWTR3	200	0	0	0	0
GRNWTR4	200	0	0	0	0
GRNWTR5	200	0.0442554	0.4091900	0	5.3002500
GRNWTR6	200	0.1742391	0.6194807	0	5.7831200
GRNWTR7	200	0.4836191	0.9088483	0	4.8789300
GRNWTR8	200	0.5985544	0.8408951	0	4.0525700
GRNWTR9	200	0.5763280	0.7258627	0	3.4344600
GRNWTR10	200	0.4995164	0.6208149	0	2.9692700
PCONC4L1	200	0	0	0	0
PCONC4L2	200	0	0	0	0
PCONC4L3	200	0.000472540	0.0048644	0	0.0592443
PCONC4L4	200	0.0101779	0.0476621	0	0.5455690
PCONC4L5	200	0.0541841	0.1062327	0	0.8719540
PCONC4L6	200	0.1157034	0.1550140	0	0.8753260
PCONC4L7	200	0.1465976	0.1655955	0	0.8452600
PCONC4L8	200	0.1386108	0.1531044	0.000033575	0.7886360
PCONC4L9	200	0.1156623	0.1341063	0.000016012	0.6952690
PCONC4L10	200	0.0929601	0.1150107	6.45387E-6	0.6113490

Table 5. PRISM/SESOIL Results for Fargo, N.D.					
Variable	N	Mean	Std Dev	Minimum	Maximum
VOLAT1	200	53.3441267	30.3965384	7.2938400	203.4380000
VOLAT2	200	12.8693754	8.5374568	0.5936580	39.4260000
VOLAT3	200	8.7013120	5.4516400	0.3993620	22.9328000
VOLAT4	200	6.7719174	4.0818907	0.3097060	16.0268000
VOLAT5	200	5.6218845	3.2604873	0.2604700	12.1244000
VOLAT6	200	4.7947490	2.7099424	0.2239770	10.1231000
VOLAT7	200	4.2009327	2.2955058	0.2013260	8.6164900
VOLAT8	200	3.7722925	2.0098767	0.1836530	7.4561300
VOLAT9	200	3.4154281	1.7885887	0.1678680	6.6995100
VOLAT10	200	3.0985116	1.6010930	0.1534900	6.0488100
GRNWTR1	200	0	0	0	0
GRNWTR2	200	0	0	0	0
GRNWTR3	200	0.0879257	0.7126118	0	8.6645500
GRNWTR4	200	1.8859029	4.2779329	0	29.0867000
GRNWTR5	200	7.8124536	7.7104430	0	28.7032000
GRNWTR6	200	11.0201498	6.3721327	0	25.7754000
GRNWTR7	200	11.0846617	4.9112845	0	23.0450000
GRNWTR8	200	10.2683333	4.2306580	0.3179050	20.5444000
GRNWTR9	200	9.3807361	3.8552791	0.2324250	18.3079000
GRNWTR10	200	8.5687498	3.5208895	0.1699000	16.3137000
PCONC4L1	200	0	0	0	0
PCONC4L2	200	0.000621511	0.0059328	0	0.0712409
PCONC4L3	200	0.0817640	0.1851874	0	1.5467200
PCONC4L4	200	0.6382280	0.5573222	0	2.6345700
PCONC4L5	200	1.2471332	0.6007071	0.0041390	2.5677100
PCONC4L6	200	1.4503265	0.4895890	0.0805248	2.3538100
PCONC4L7	200	1.3996711	0.4316642	0.0674375	2.2083800
PCONC4L8	200	1.2910424	0.4060135	0.0493299	2.1079200
PCONC4L9	200	1.1839926	0.3867622	0.0360646	2.0101500
PCONC4L10	200	1.0859063	0.3690826	0.0263618	1.9167600

X. FIGURE CAPTIONS

Fig. 1. Flowchart of steps for the PRISM/SESOIL model.

Fig. 2. Relative frequency distribution for mass flux to groundwater during year 2 at the Oak Ridge, Tenn., site.

Fig. 3. Relative frequency distribution for mass flux volatilized during year 1 at the Oak Ridge, Tenn., site.

Fig. 4. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 2 at the Oak Ridge, Tenn., site.

Fig. 5. Relative frequency distribution for mass flux to groundwater during year 8 at the Fresno, Calif., site.

Fig. 6. Relative frequency distribution for mass flux volatilized during year 1 at the Fresno, Calif., site.

Fig. 7. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 7 at the Fresno, Calif., site.

Fig. 8. Relative frequency distribution for mass flux to groundwater during year 7 at the Fargo, N.D., site.

Fig. 9. Relative frequency distribution for mass flux volatilized during year 1 at the Fargo, N.D., site.

Fig. 10. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 6 at the Fargo, N.D., site.

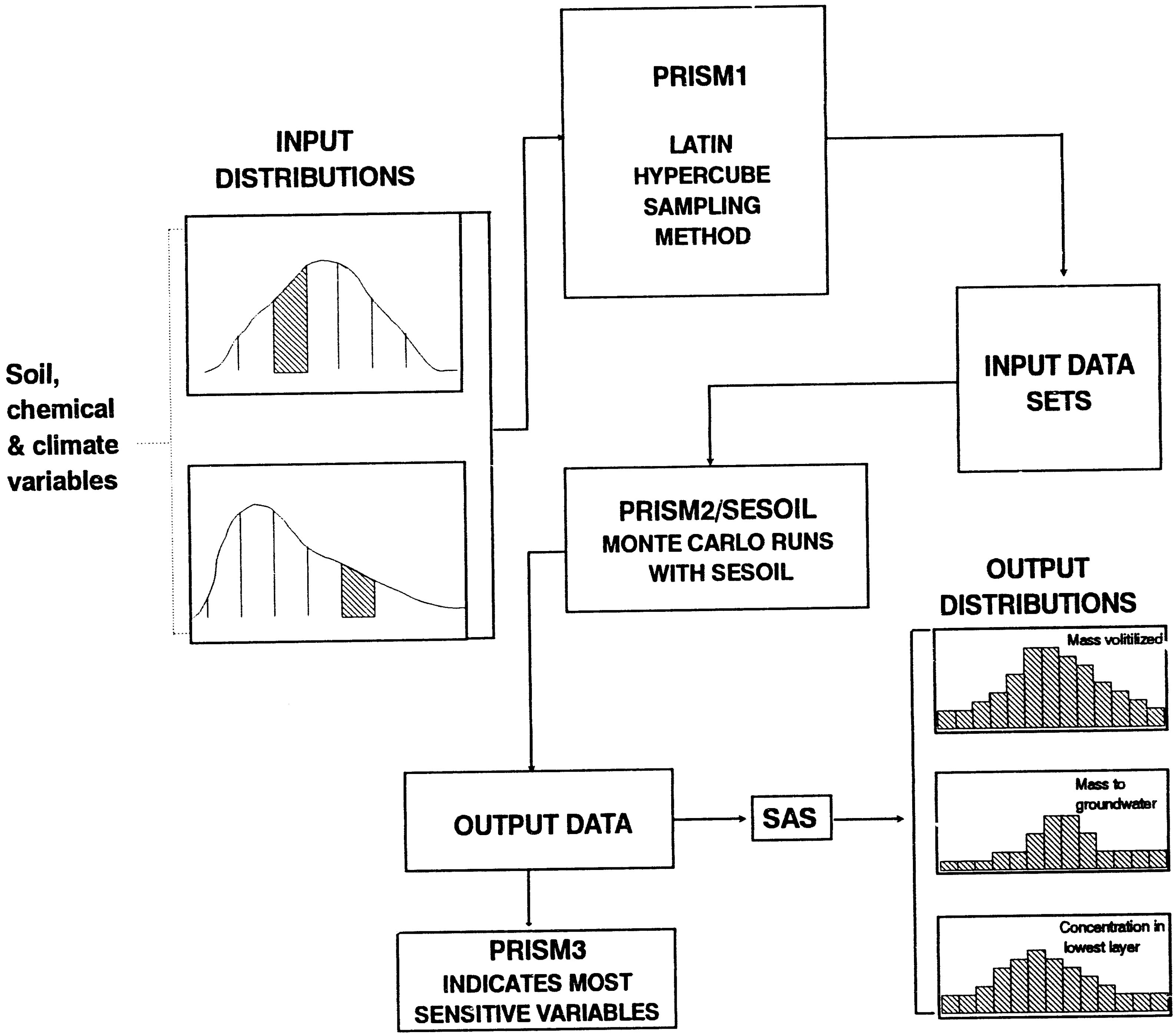

Fig. 1. Flowchart of steps for the PRISM/SESOIL model

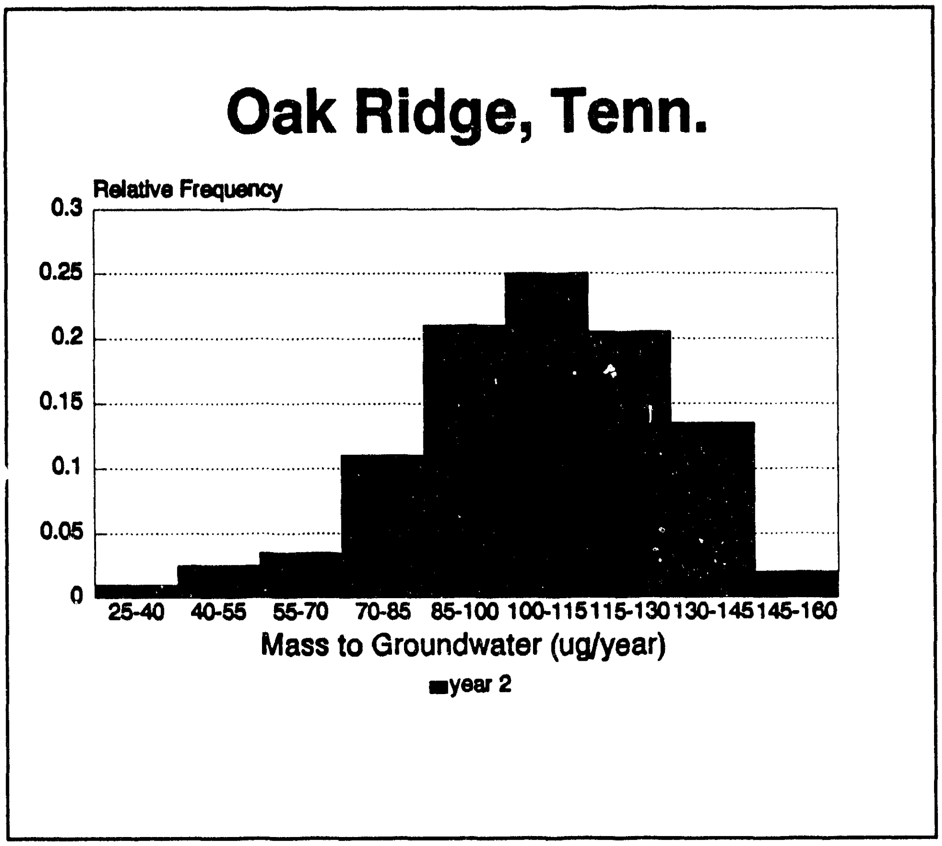

Fig 2. Relative frequency distribution for mass flux to groundwater during year 2 at the Oak Ridge, Tenn., site

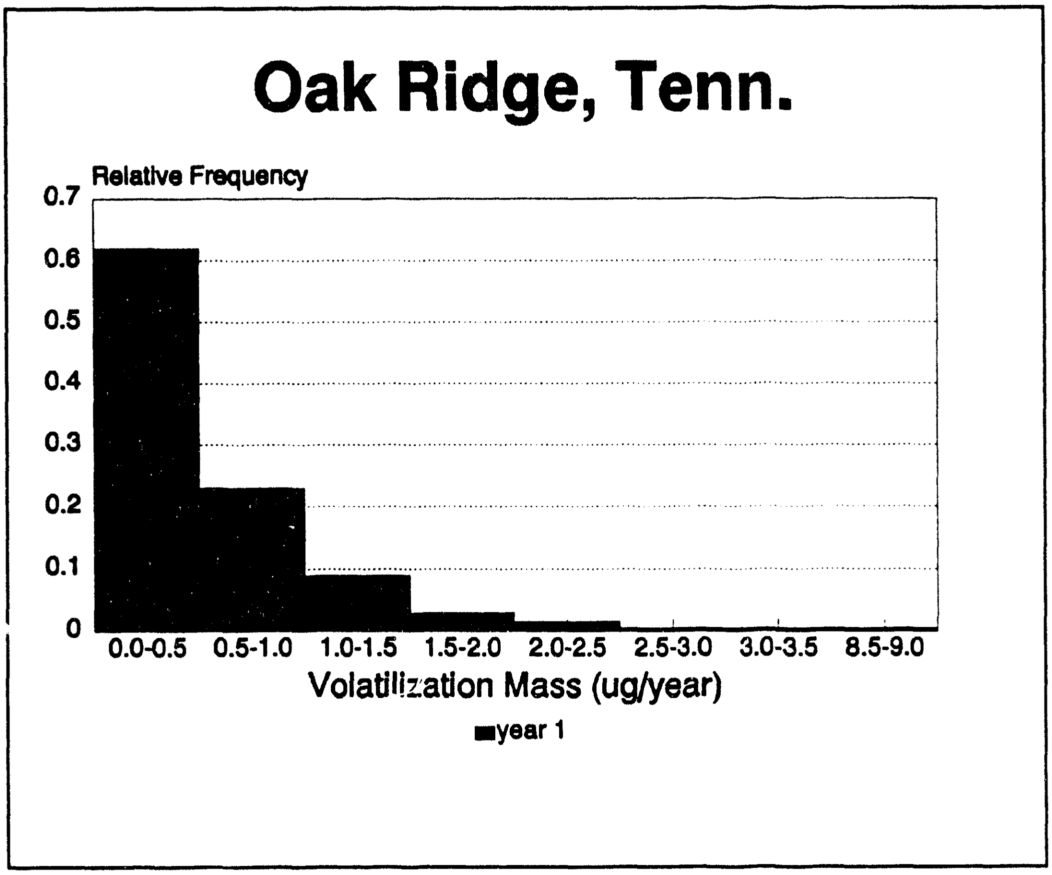

Fig. 3. Relative frequency distribution for mass flux volatilized during year 1 at the Oak Ridge, Tenn., site

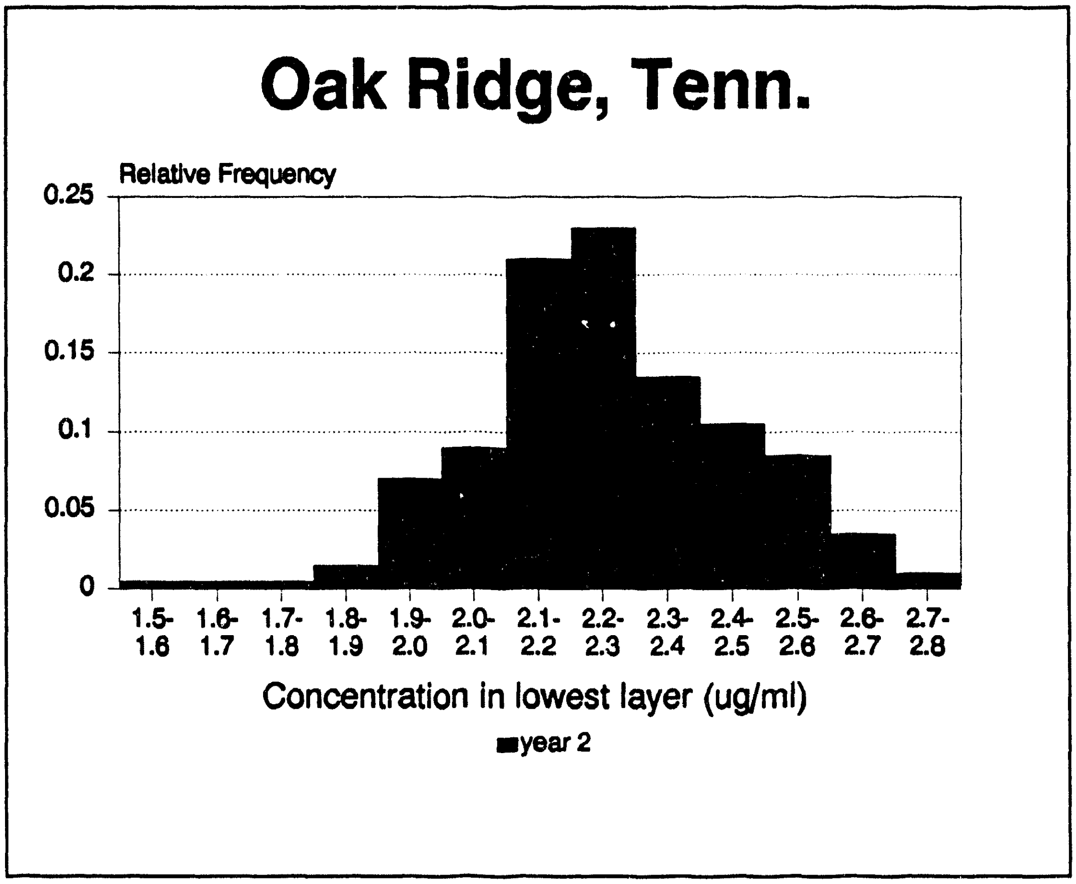

Fig.4. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 2 at the Oak Ridge, Tenn., site

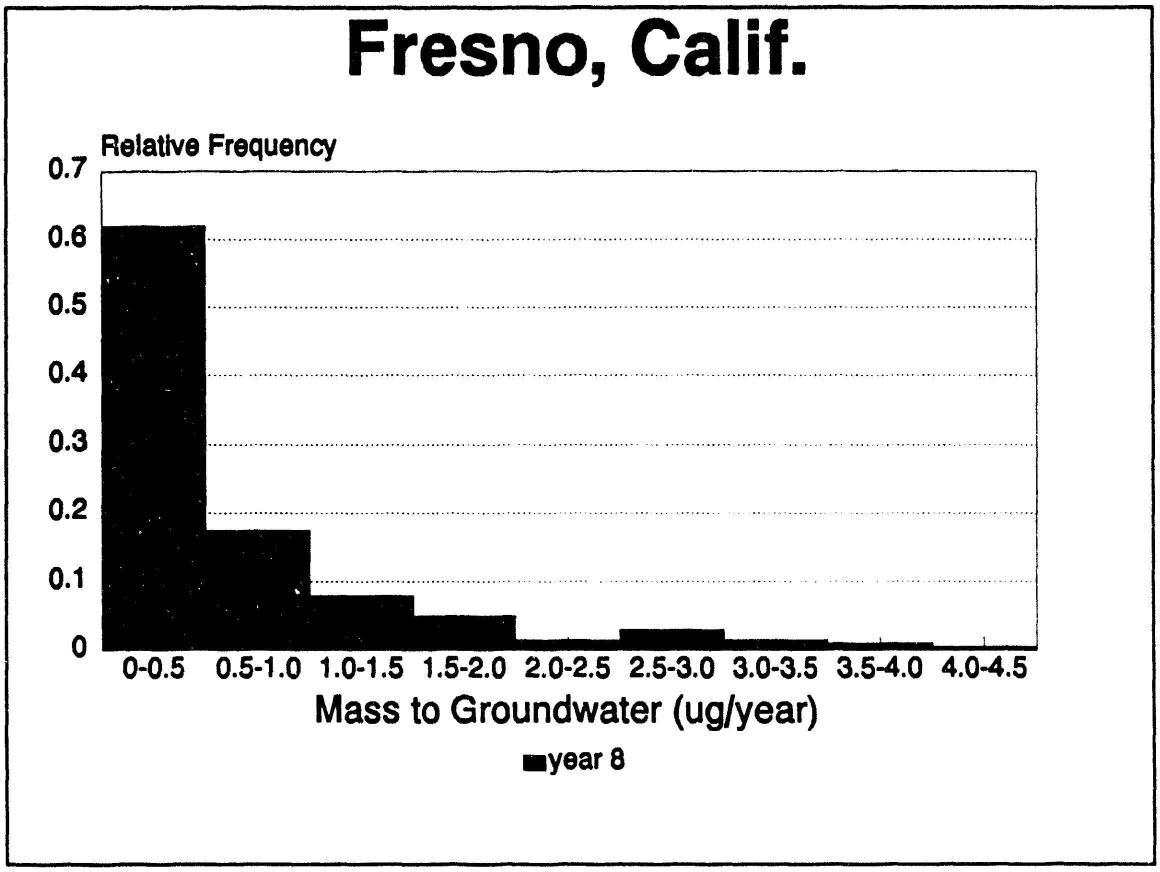

Fig. 5. Relative frequency distribution for mass flux to groundwater during year 8 at the Fresno, Calif., site

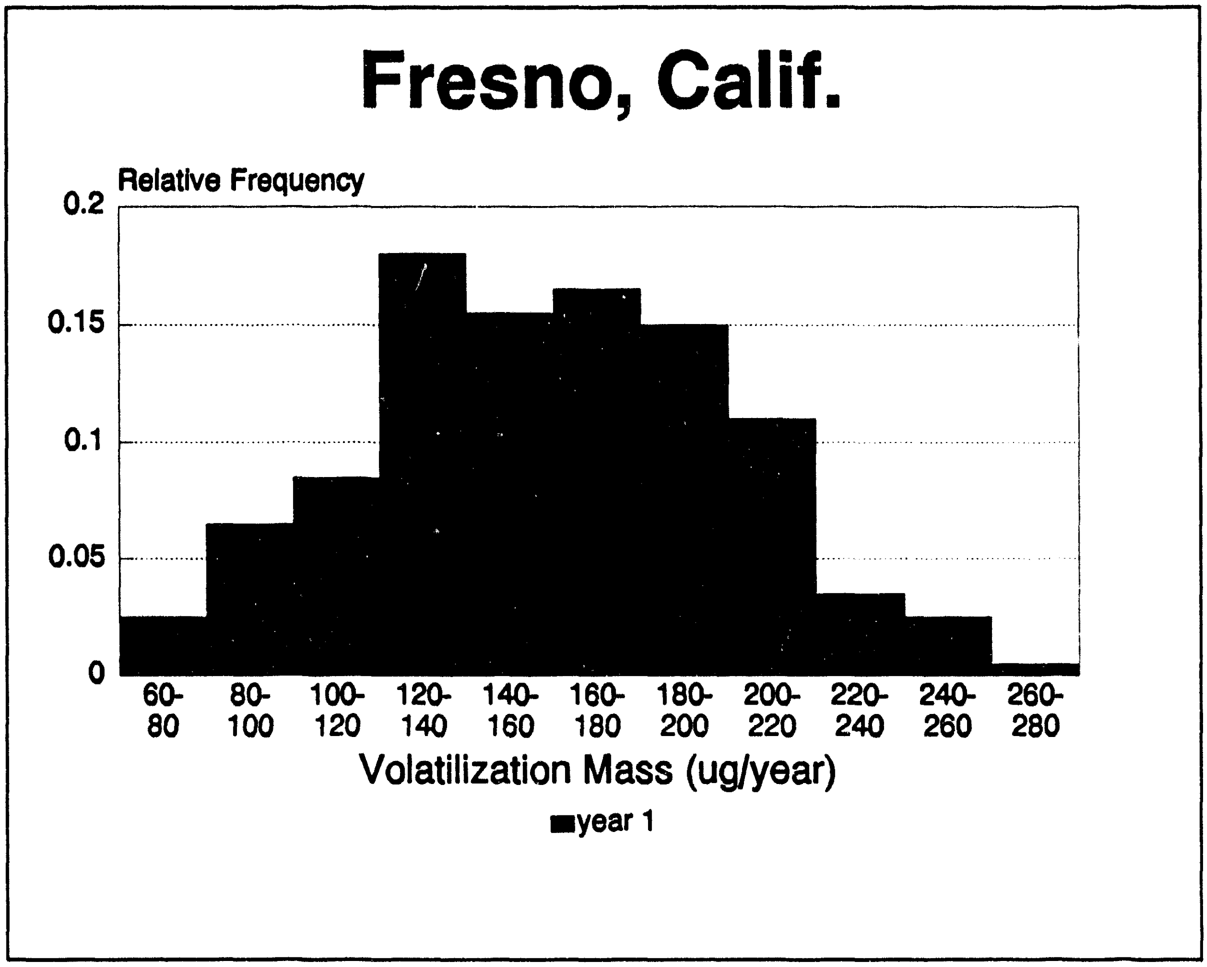

Fig. 6. Relative frequency distribution for mass flux volatilized during year 1 at the Fresno, Calif., site

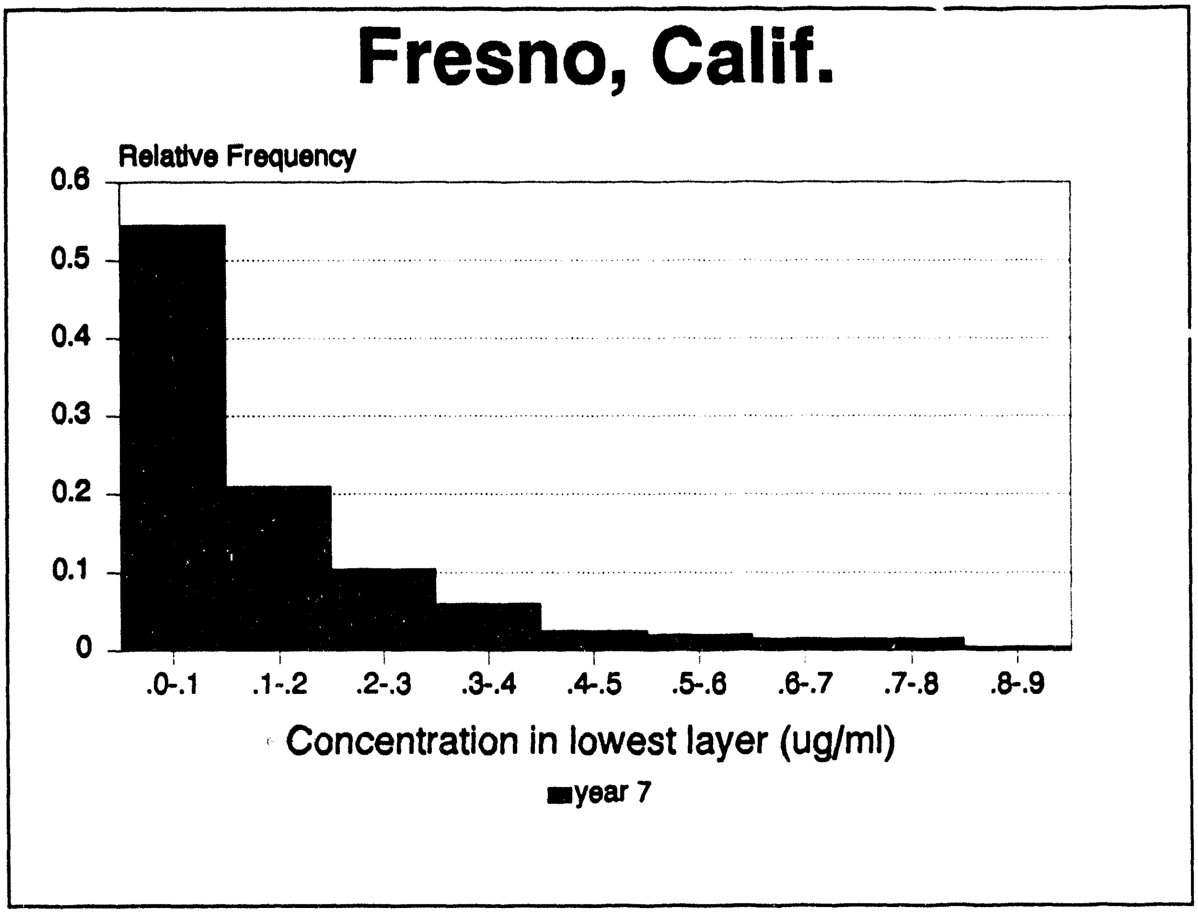

Fig. 7. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 7 at the Fresno, Calif., site

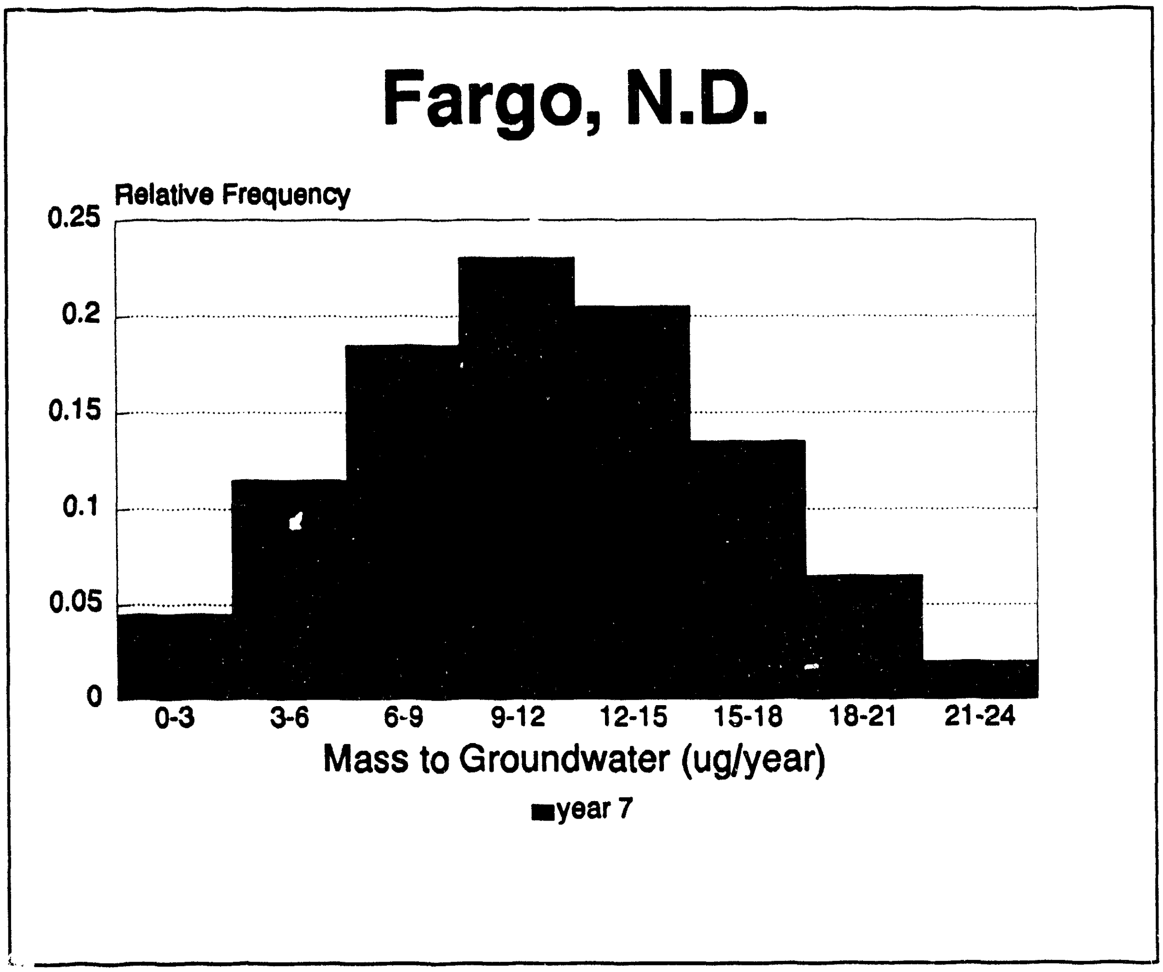

Fig. 8. Relative frequency distribution for mass flux to groundwater during year 7 at the Fargo, N.D., site

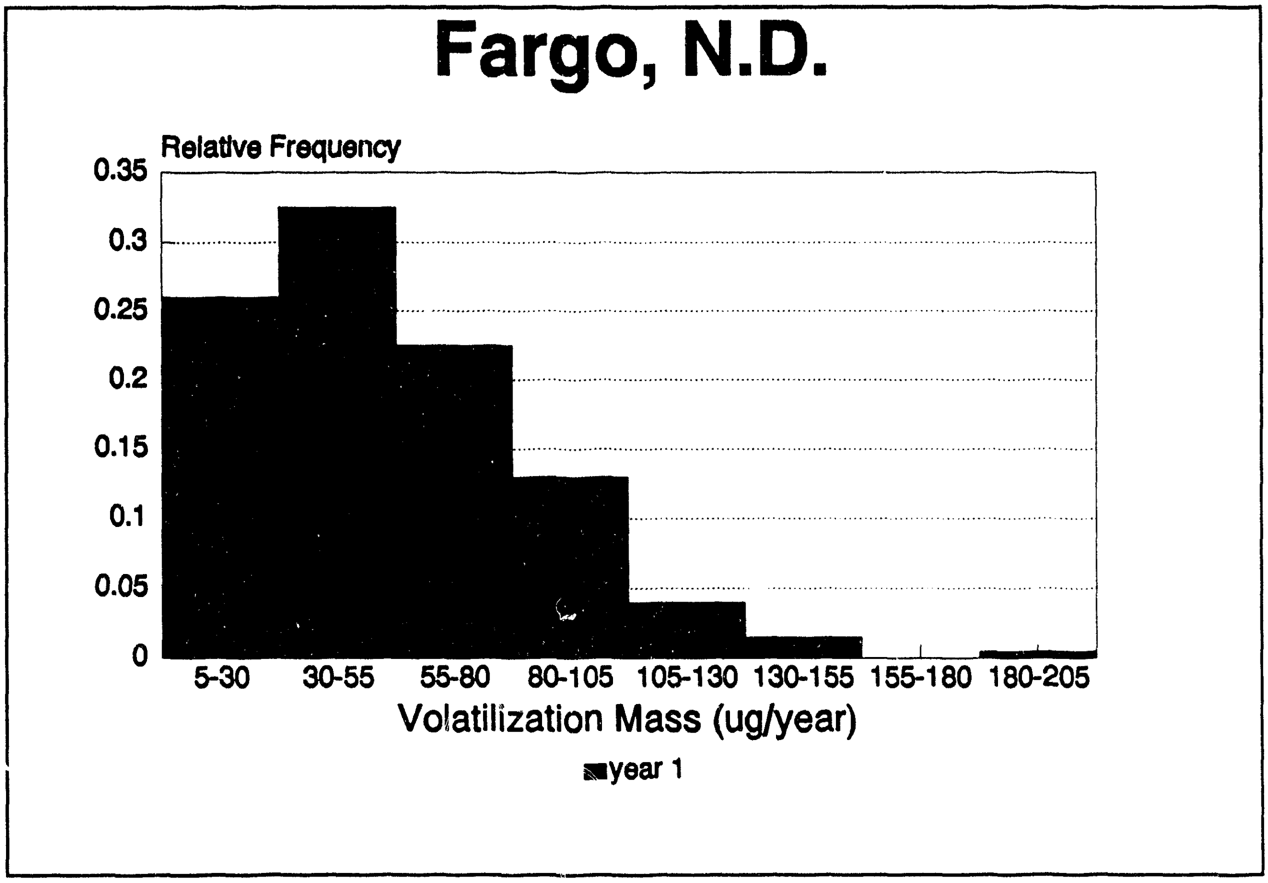

Fig. 9. Relative frequency distribution for mass flux volatilized during year 1 at the Fargo, N.D., site

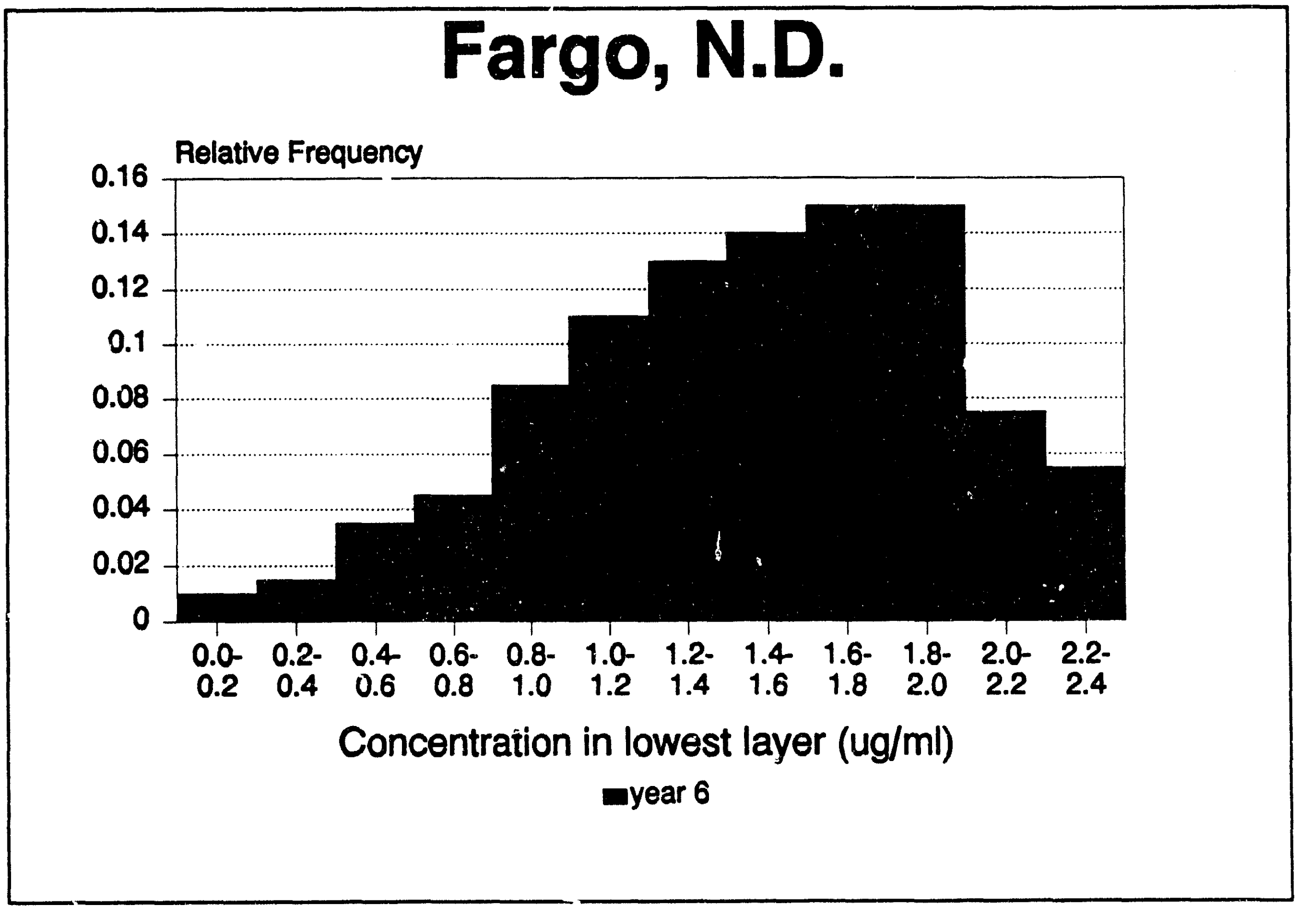

Fig. 10. Relative frequency distribution for average dissolved pollutant concentration in the lowest sublayer for year 6 at the Fargo, N.D., site

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