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Simulation of Organic Chemical Movement in Hawaii Soils with PRZM: 3. Calibration[1]

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ABSTRACT: This is the third and final part of a multipart paper reporting testing of the EPA's Pesticide Root Zone Model (PRZM) using data from Hawaii. PRZM is a dynamic-conceptual pesticide leaching model. In the first and second parts of the paper results were reported for predicted pesticide movement based upon preliminary PRZM simulations. In this part of the paper a trial-and-error calibration of PRZM is reported for a site in Hawaii. Performance results from the model calibration exercise are quite poor, illustrating the need for multicriteria evaluation procedures.

IN THE FIRST TWO PARTS of this multipart paper we (Loague et al. 1989*a*,*b*) conducted an initial qualitative evaluation of the Environmental Protection Agency (EPA) Pesticide Root Zone Model (PRZM) using deep DBCP (1,2-dibromo-3-chloropropane) and EDB (ethylene dibromide) concentration profiles in Hawaii. In our earlier work we applied PRZM well beyond its intended (near-surface) range to determine whether the model could provide reasonable estimates of peak concentrations for leaching pesticides in highly structured soil and fractured rock. Here in the final part of the paper the performance of PRZM is quantitatively evaluated for a series of calibration simulations. A preliminary version of the work reported here was first presented by Loague and Green (1990).

Pesticide Root Zone Model (PRZM)

PRZM, as used in this study, has two components for the unsaturated near-surface: (1) a water-balance algorithm, and (2) a chemical-transport algorithm. The water-balance algorithm is made up of three simple equations that partition water within and between the surface, the active root zone, and the remainder of the unsaturated zone. The elements of the water balance include precipitation, interception, evapotranspiration, run-off, and recharge. The chemical-transport algorithm is an implicit finite-difference approximation to the one-dimensional advection-dispersion equation. Solution of the transport equation requires values for soil-water content and velocity throughout the soil profile at each time step. This information is obtained, based upon major simplifying assumptions, from the water-balance algorithm. The form of the advection-dispersion equation employed here includes the effects of sorption and degradation. A complete description of PRZM is outlined by the model developers (Carsel et al. 1984). Short-term volatilization effects, which cannot be simulated with PRZM, but which are included in the simulations reported in this study, were preprocessed with a separate model as described by Loague et al. (1989*a*).

Pineapple Field 4201 Revisited

The data set used in this study is for the site 4201a located within a single pineapple field on the Hawaiian island of Oahu. Field 4201 is near Mililani within the Pearl Harbor Watershed (see Figure 1). A description of the general characteristics of field 4201 has been given earlier (Loague et al. 1989*a*). Observed EDB concentration profiles for 4201a for

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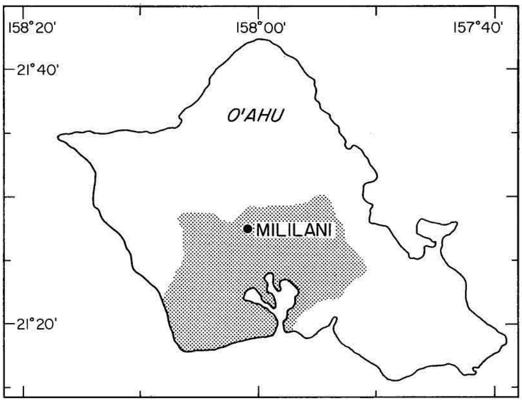

FIGURE 1. Island of Oahu with the Pearl Harbor Watershed shaded.

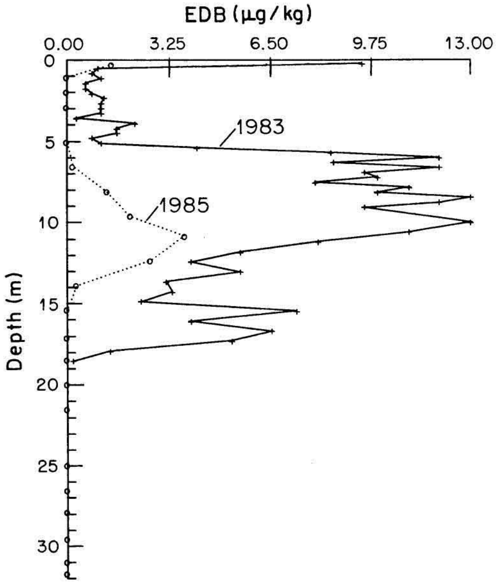

FIGURE 2. Observed EDB concentration profiles for 4201a.

1983 and 1985 are shown in Figure 2. The parameter estimates needed for PRZM for the 4201a site were presented in the first two parts of this paper (Loague et al. 1989*a*, *b*). The base case simulation for this study for 4201a is the case H simulation described in Loague et al. (1989*b*). Observed versus predicted EDB concentration profiles for 4201a for 1983 and 1985 for the base case simulations are shown in Figure 3.

Model Performance Evaluation

In general, with the exception of research models used in concept development, solute transport models are used to predict the fate of chemicals. A model used to predict should first be calibrated and validated. The concepts of calibration, validation, and prediction, relative to solute transport modeling, as described here, are reviewed by Loague and Green (1991). The principles are generally transferable to all mathematical simulation models. For solute transport models, field-measured concentration profiles or summary variables can be used to calibrate a model at a given time by adjusting parameters until an acceptable simulation is achieved. Once this fit is obtained another simulation is performed for a later time and compared with a second set of measured data. If the second simulation is also acceptable, the model may be considered validated. Model parameters are not adjusted, based on field data, during validation. If the parameters are adjusted, for simulations subsequent to calibration, then the effort is not a validation but a recalibration. The level of model performance should be the same for the split sample calibration and validation periods. The idealized calibration and validation procedures are shown schematically in Figure 4.

Assessment procedures that combine more than one measure of model performance are useful for conducting comparative evaluations between competing models. A comparison of summary statistics (e.g., mean and standard deviation) for observed and predicted summary variables gleaned from concentration profiles is one statistical criterion for evaluation of model performance. Examples of summary variables for a leaching pesticide include (1) total mass, (2) center of mass, (3) peak concentration, (4) time for a critical concentration to leach to a depth of interest, (5) depth-to-peak concentration, and (6) depth of the leaching front.

Analysis of residual errors also can be used to evaluate statistically the performance of pesticide leaching models by characterizing, for example, systematic under- or over-prediction. Several such measures are available;

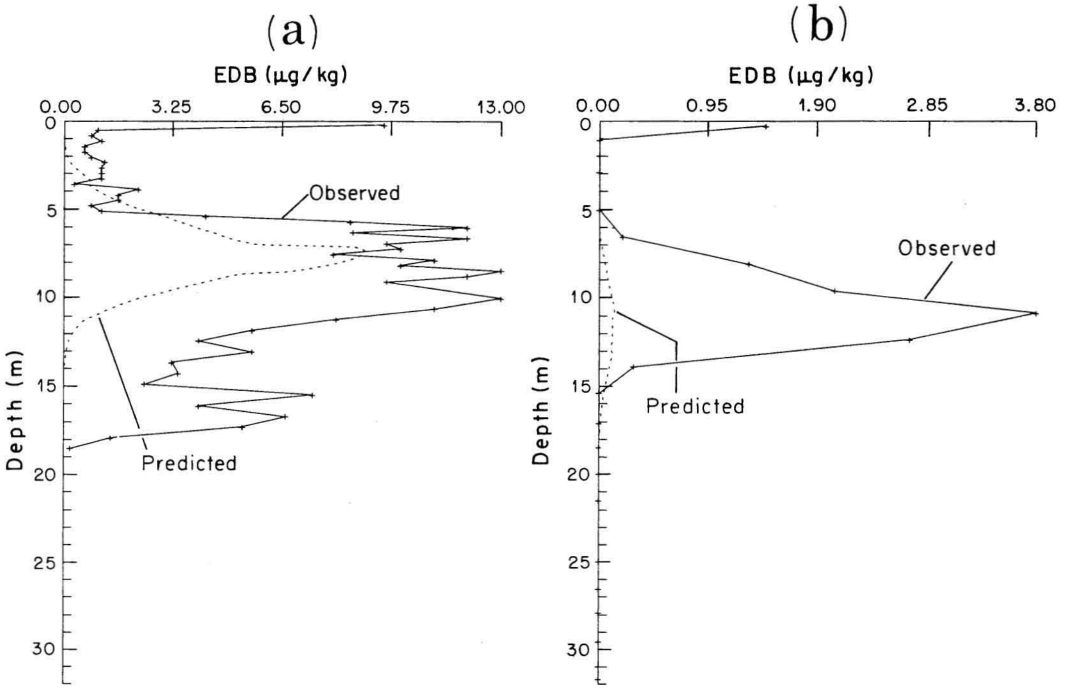

FIGURE 3. Observed versus predicted EDB concentration profiles for 4201a. The predicted profiles are the base case simulations: *a*, 1983; *b*, 1985.

these include, for example, maximum error (ME), root mean square error (RMSE), coefficient of determination (CD), modeling efficiency (EF), and coefficient of residual mass (CRM). The mathematical expressions that describe these measures of analysis are given in Table 1. The lower limit for ME, RMSE, and CD statistics is zero. The maximum value for EF is one. Both EF and CRM can become negative. If EF is less than zero the model-predicted values are worse than simply using the observed mean. CD is a measure of the proportion of the total variance of observed data explained by the predicted data. Several of the above statistics are sensitive to a few large errors, especially in small data sets.

Each of the five statistical criteria given here are (of course) not of equal importance or, depending upon the questions being asked, even suitable for all model evaluations. For example, when comparing observed versus predicted profile characteristics one might rank the statistics, in order of most usefulness, as RMSE > EF > CRM > ME > CD. In fact, the CD statistic may even be inappropriate for evaluating the characteristics of predicted concentration profiles; it would probably be more useful in comparing predicted and observed summary variables for different locations or perhaps at different times. For the purpose of this illustrative example, however, where no final judgment on model performance is being made, all the statistics are included. To the best of my knowledge, standards and even the relative usefulness of the statistics listed here (as well as others) have not yet been established for the various applications in which they might be used.

Statistical measures of model performance can have serious limitations. Graphical displays are often useful for showing trends, types of errors, and distribution patterns not identified with statistical measures. Several types of graphical display are possible; see for example Loague and Green (1991).

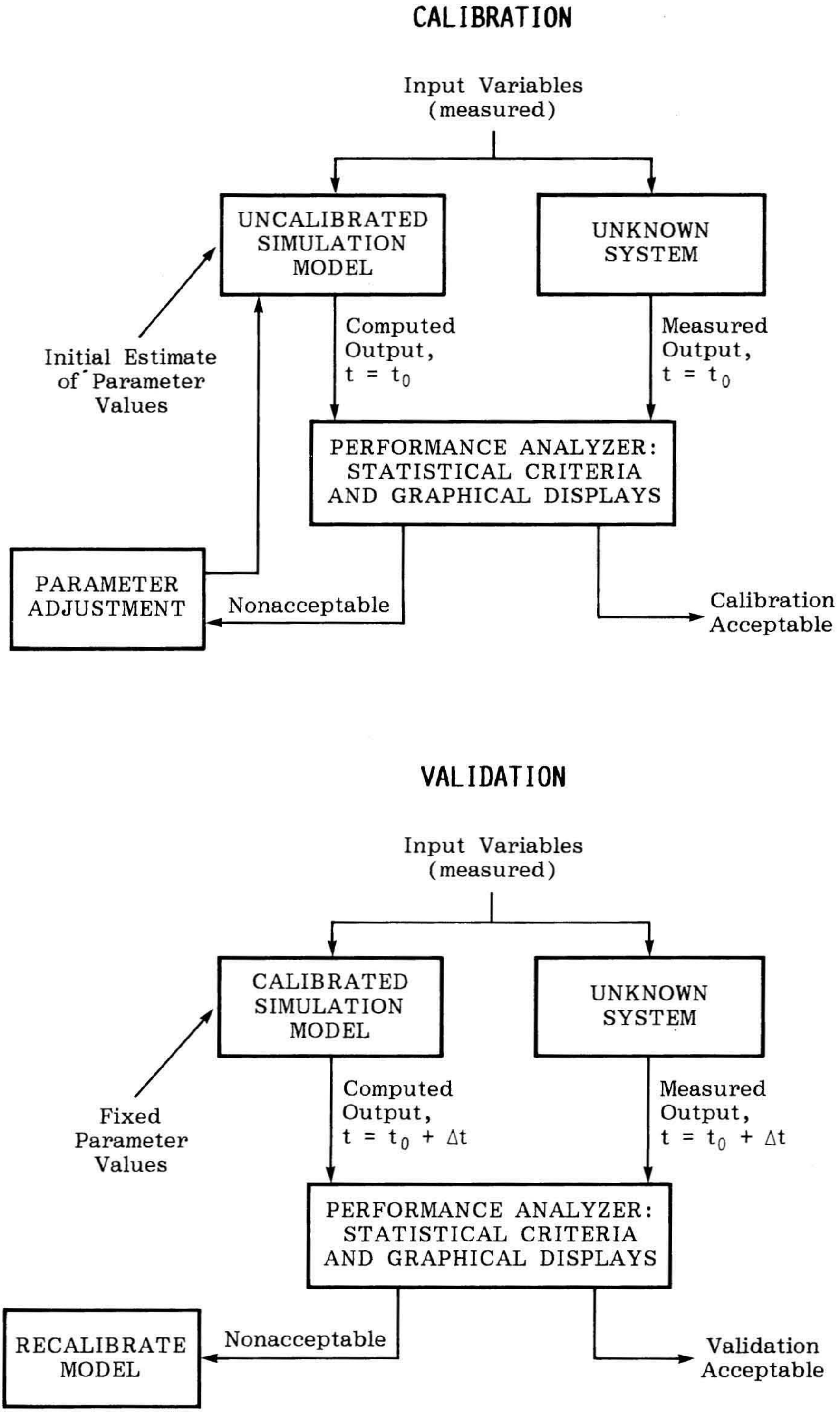

FIGURE 4. Schematic of calibration and validation procedures.

TABLE 1

MEASURES FOR ANALYSIS OF RESIDUAL ERRORS (LOAGUE AND GREEN 1991)

Maximum error

$$\mathrm{ME} = \mathrm{Max}|P_i - O_i|\Big|_{i=1}^{n}$$

Root mean square error

$$\mathrm{RMSE} = \left[\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}\right]^{0.5} \cdot \frac{100}{\bar{O}}$$

Coefficient of residual mass

$$\mathrm{CRM} = \frac{\sum_{i=1}^{n} O_i - \sum_{i=1} P_i}{\sum_{i=1}^{n} O_i}$$

Coefficient of determination

$$\mathrm{CD} = \frac{\sum_{i-1}^{n}(O_i - \bar{O})^2}{\sum_{i=1}^{n}(P_i - \bar{O})^2}$$

Modeling efficiency

$$\mathrm{EF} = \frac{\sum_{i=1}^{n}(O_i - \bar{O})^2 - \sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2}$$

P_i = predicted values; O_i = observed values; $\bar{O}$ = mean of the observed data; n = number of samples.

PROCEDURE

A series of 120 PRZM simulations was performed for 4201a to evaluate the ability of the model to predict the EDB concentration profiles for September 1983 and September 1985. These simulations, summarized as cases 1–120 in Table 2, consist of trial-and-error adjustments of two parameters: (1) the hydrodynamic dispersion coefficient, and (2) the pesticide decay rate. In cases 1–60, decay is confined to the upper 5.5 m. The dispersion coefficient in cases 1–12 increases with depth; for cases 13 through 60 it remains constant. In cases 61–120, decay is not confined to the top layer. Dispersion rates remain in the same range for cases 61–120 as for cases 1–60. The 120 cases for 4201a are certainly not all the possible combinations for the two parameters used here to calibrate PRZM. They are more than sufficient, however, for this example.

In this study all five of the statistics (discussed above) are given equal weight and included in the examples. The results for each case are ranked from 1 to 120 to infer model performance. To combine the statistics for a multicriteria evaluation, a two-step procedure is used: (1) sum the ranked positions for each of the five statistics for each individual case and (2) rank the summed "averages." The average procedure is employed for the 1983 and 1985 data for 4201a. The "total average" is based upon summing the 1983 and 1985 ranked averages for each case and ranking them. The same procedures are employed, for the profile characteristic results, as are described above for the statistical criteria results. The P_i and O_i values for the statistics (see Table 1) are the predicted and observed EDB concentrations at different depths for a given case profile.

RESULTS

In Table 3 the concentration profile results for the 120 cases for 4201a are summarized in terms of the five statistical criteria (ME, RMSE, CRM, CD, EF) and two summary variables (depth-to-peak, peak concentration) for 1983 and for 1985. In Tables 4–5 the cases are ranked for 1983 and 1985 on the basis of the statistical criteria and the two summary variables. The average rankings given in Tables 4–5 are simple averages for the individual statistical and profile characteristic results.

Plots of observed versus predicted concentration profiles for the best-ranked cases are shown in Figures 5 through 12. Figures 5 and 7 contain profiles of the best-ranked cases based on statistical criteria for 1983 and 1985. Figures 6 and 8 contain profiles of the best-ranked cases based on summary variables for 1983 and 1985. Figures 9 and 11 show the best averaged cases based on statistical criteria for 1983 and 1985. Figures 10 and 12 show the best averaged cases based on summary variables for 1983 and 1985.

TABLE 2

SUMMARY OF PRZM SIMULATIONS

	DISPERSION (cm^2/day)*				DECAY RATE (day^{-1})			
CASE	LAYER 1**	LAYER 2	LAYER 3	LAYER 4	LAYER 1	LAYER 2	LAYER 3	LAYER 4
Base***	13	13	13	13	0	0	0	0
1	13	25	50	100	0.0025	0	0	0
2	13	25	50	100	0.003	0	0	0
3	13	25	50	100	0.0035	0	0	0
4	13	25	50	100	0.004	0	0	0
5	13	25	50	100	0.0045	0	0	0
6	13	25	50	100	0.005	0	0	0
7	13	25	50	100	0.0055	0	0	0
8	13	25	50	100	0.006	0	0	0
9	13	25	50	100	0.0065	0	0	0
10	13	25	50	100	0.007	0	0	0
11	13	25	50	100	0.0075	0	0	0
12	13	25	50	100	0.008	0	0	0
13	13	13	13	13	0.0025	0	0	0
14	13	13	13	13	0.003	0	0	0
15	13	13	13	13	0.0035	0	0	0
16	13	13	13	13	0.004	0	0	0
17	13	13	13	13	0.0045	0	0	0
18	13	13	13	13	0.005	0	0	0
19	13	13	13	13	0.0055	0	0	0
20	13	13	13	13	0.006	0	0	0
21	13	13	13	13	0.0065	0	0	0
22	13	13	13	13	0.007	0	0	0
23	13	13	13	13	0.0075	0	0	0
24	13	13	13	13	0.008	0	0	0
25	25	25	25	25	0.0025	0	0	0
26	25	25	25	25	0.003	0	0	0
27	25	25	25	25	0.0035	0	0	0
28	25	25	25	25	0.004	0	0	0
29	25	25	25	25	0.0045	0	0	0
30	25	25	25	25	0.005	0	0	0
31	25	25	25	25	0.0055	0	0	0
32	25	25	25	25	0.006	0	0	0
33	25	25	25	25	0.0065	0	0	0
34	25	25	25	25	0.007	0	0	0
35	25	25	25	25	0.0075	0	0	0
36	25	25	25	25	0.008	0	0	0
37	50	50	50	50	0.0025	0	0	0
38	50	50	50	50	0.003	0	0	0
39	50	50	50	50	0.0035	0	0	0
40	50	50	50	50	0.004	0	0	0
41	50	50	50	50	0.0045	0	0	0
42	50	50	50	50	0.005	0	0	0
43	50	50	50	50	0.0055	0	0	0
44	50	50	50	50	0.006	0	0	0
45	50	50	50	50	0.0065	0	0	0
46	50	50	50	50	0.007	0	0	0
47	50	50	50	50	0.0075	0	0	0
48	50	50	50	50	0.008	0	0	0
49	100	100	100	100	0.0025	0	0	0
50	100	100	100	100	0.003	0	0	0
51	100	100	100	100	0.0035	0	0	0
52	100	100	100	100	0.004	0	0	0

TABLE 2 (continued)

	DISPERSION (cm^2/day)*				DECAY RATE (day^{-1})			
CASE	LAYER 1**	LAYER 2	LAYER 3	LAYER 4	LAYER 1	LAYER 2	LAYER 3	LAYER 4
53	100	100	100	100	0.0045	0	0	0
54	100	100	100	100	0.005	0	0	0
55	100	100	100	100	0.0055	0	0	0
56	100	100	100	100	0.006	0	0	0
57	100	100	100	100	0.0065	0	0	0
58	100	100	100	100	0.007	0	0	0
59	100	100	100	100	0.0075	0	0	0
60	100	100	100	100	0.008	0	0	0
61	13	13	13	13	0.0025	0.0025	0.0025	0.0025
62	13	13	13	13	0.003	0.003	0.003	0.003
63	13	13	13	13	0.0035	0.0035	0.0035	0.0035
64	13	13	13	13	0.004	0.004	0.004	0.004
65	13	13	13	13	0.0045	0.0045	0.0045	0.0045
66	13	13	13	13	0.005	0.005	0.005	0.005
67	13	13	13	13	0.0055	0.0055	0.0055	0.0055
68	13	13	13	13	0.006	0.006	0.006	0.006
69	13	13	13	13	0.0065	0.0065	0.0065	0.0065
70	13	13	13	13	0.007	0.007	0.007	0.007
71	13	13	13	13	0.0075	0.0075	0.0075	0.0075
72	13	13	13	13	0.008	0.008	0.008	0.008
73	13	25	50	100	0.0025	0.0025	0.0025	0.0025
74	13	25	50	100	0.003	0.003	0.003	0.003
75	13	25	50	100	0.0035	0.0035	0.0035	0.0035
76	13	25	50	100	0.004	0.004	0.004	0.004
77	13	25	50	100	0.0045	0.0045	0.0045	0.0045
78	13	25	50	100	0.005	0.005	0.005	0.005
79	13	25	50	100	0.0055	0.0055	0.0055	0.0055
80	13	25	50	100	0.006	0.006	0.006	0.006
81	13	25	50	100	0.0065	0.0065	0.0065	0.0065
82	13	25	50	100	0.007	0.007	0.007	0.007
83	13	25	50	100	0.0075	0.0075	0.0075	0.0075
84	13	25	50	100	0.008	0.008	0.008	0.008
85	13	25	50	100	0.0025	0.002	0.0015	0.001
86	13	25	50	100	0.003	0.0024	0.0018	0.0012
87	13	25	50	100	0.0035	0.0028	0.0021	0.0014
88	13	25	50	100	0.004	0.0032	0.0024	0.0016
89	13	25	50	100	0.0045	0.0036	0.0027	0.0018
90	13	25	50	100	0.005	0.004	0.003	0.082
91	13	25	50	100	0.0055	0.0044	0.0033	0.0022
92	13	25	50	100	0.006	0.0048	0.0036	0.0024
93	13	25	50	100	0.0065	0.0052	0.0039	0.0026
94	13	25	50	100	0.007	0.0056	0.0042	0.0028
95	13	25	50	100	0.0075	0.006	0.0045	0.003
96	13	25	50	100	0.008	0.0064	0.0048	0.0032
97	13	13	13	13	0.0025	0.0025	0	0
98	13	13	13	13	0.003	0.003	0	0
99	13	13	13	13	0.0035	0.0035	0	0
100	13	13	13	13	0.004	0.004	0	0
101	13	13	13	13	0.0045	0.0045	0	0
102	13	13	13	13	0.005	0.005	0	0
103	13	13	13	13	0.0055	0.0055	0	0
104	13	13	13	13	0.006	0.006	0	0
105	13	13	13	13	0.0065	0.0065	0	0
106	13	13	13	13	0.007	0.007	0	0
107	13	13	13	13	0.0075	0.0075	0	0

TABLE 2 (continued)

	DISPERSION (cm^2/day)*				DECAY RATE (day^{-1})			
CASE	LAYER 1**	LAYER 2	LAYER 3	LAYER 4	LAYER 1	LAYER 2	LAYER 3	LAYER 4
108	13	13	13	13	0.008	0.008	0	0
109	13	25	50	100	0.0025	0.0025	0	0
110	13	25	50	100	0.003	0.003	0	0
111	13	25	50	100	0.0035	0.0035	0	0
112	13	25	50	100	0.004	0.004	0	0
113	13	25	50	100	0.0045	0.0045	0	0
114	13	25	50	100	0.005	0.005	0	0
115	13	25	50	100	0.0055	0.0055	0	0
116	13	25	50	100	0.006	0.006	0	0
117	13	25	50	100	0.0065	0.0065	0	0
118	13	25	50	100	0.007	0.007	0	0
119	13	25	50	100	0.0075	0.0075	0	0
120	13	25	50	100	0.008	0.008	0	0

* 1.0 cm^2/day = 1.16×10^{-9} m^2/s.

** 4201a: Layer 1 = 0–5.5 m
Layer 2 = 5.5–11
Layer 3 = 11–20
Layer 4 = 20–32

*** Loague et al. (1989*a*,*b*).

Perusal of Table 3 leads to the following generalized comments about the statistical criteria and summary variables for 4201a for 1983 and 1985: (1) Overall model performance is quite poor, as indicated by the low EF values, which exceed zero only slightly for some cases; (2) Model performance for 1983 is superior to that for 1985.

Perusal of Table 4 leads to the following generalized comments about the ranked and average rankings based upon the statistical results for 4201a for 1983 and 1985: (1) The best cases for 4201a for 1983 (ME, 55; RMSE, 58; CRM, 7; CD, 79; EF, 58) have larger hydrodynamic dispersion coefficient values than the base case. Case 58 is the highest ranked for both RMSE and EF; (2) Decay rates for the highest ranked cases for 4201a for 1983 are in the moderate to high range of the rates tested; (3) The best cases for 4201a for 1985 (74, 87, 111) all have hydrodynamic dispersion coefficient values that change with depth; (4) Decay rates for the best cases for 4201a for 1985 are lower than the base case; (5) The highest ranked (average) case for 1983 for 4201a (58) is ranked 78 for 1985; the highest ranked (average) case for 1985 for 4201a (87) is ranked 76 for 1983; (6) The highest ranked results for 4201a in 1983 and 1985 are for cases with higher hydrodynamic dispersion coefficient values than the base case; (7) For the average rankings the best results in 1983 are achieved with decay rates higher than the base case; the best results in 1985 are achieved with decay rates lower than the base case.

Perusal of Table 5 leads to the following generalized comments about the ranked and average rankings of the summary variables for 4201a for 1983 and 1985: (1) The best cases for 4201a for 1983 for the depth-to-peak criterion (12, 24, 32, 33, 39), where the observed depth-to-peak is best represented by the predicted depth-to-peak estimate, have higher hydrodynamic dispersion coefficient values and larger decay rates than the base case; (2) The best case for the peak concentration criterion for 4201a for 1983 (11) has a higher decay rate than the base case; (3) The best-ranked cases based on the depth-to-peak criterion for 1985 cover a wide range of values for both input parameters for 4201a (6–17, 73–96); (4) The best-ranked case based on peak concentration criterion for 4201a for

TABLE 3

SUMMARY OF PREDICTED PROFILE CHARACTERISTICS AND STATISTICS FOR CONCENTRATION VERSUS DEPTH DATA FOR 4201a

	1983							1985						
	PROFILE CHARACTERISTICS		STATISTICS*					PROFILE CHARACTERISTICS		STATISTICS				
CASE	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF
Base	7.4	8.95	10.71	86	0.62	1.02	−0.13	7.2	8.98	5.56	375	−0.61	0.30	−2.78
1	7.8	107.30	96.40	661	−3.25	0.01	−65.68	13.1	63.17	59.71	3656	−18.18	0.00	−358.50
2	7.9	86.05	74.82	509	−2.35	0.02	−38.48	13.2	50.23	47.97	2884	−14.17	0.00	−222.75
3	8.0	69.17	57.94	390	−1.65	0.03	−22.17	13.2	40.09	38.65	2285	−11.06	0.01	−139.44
4	8.0	55.85	45.15	297	−1.11	0.06	−12.45	13.2	32.10	31.21	1817	−8.64	0.01	−87.82
5	8.0	45.16	34.84	225	−0.68	0.09	−6.73	13.5	25.88	25.26	1450	−6.74	0.02	−55.55
6	8.0	30.03	20.30	135	−0.24	0.19	−1.80	11.0	17.99	13.87	963	−5.23	0.03	−23.96
7	8.1	24.28	14.55	102	0.01	0.30	−0.60	11.0	14.24	11.20	757	−4.02	0.05	−14.40
8	8.1	19.70	10.01	82	0.20	0.44	−0.03	11.0	11.31	9.05	596	−3.07	0.09	−8.54
9	8.1	16.02	9.50	74	0.36	0.61	0.16	11.0	9.03	7.33	471	−2.31	0.13	−4.96
10	8.2	13.07	9.7	74	0.48	0.76	0.16	11.0	7.23	5.94	375	−1.70	0.21	−2.78
11	8.2	10.68	10.26	79	0.58	0.87	0.05	11.0	5.82	4.82	303	−1.21	0.32	−1.47
12	8.3	8.75	10.68	85	0.66	0.92	−0.10	11.0	4.69	3.91	251	−0.81	0.50	−0.70
13	7.7	91.7	83.32	582	−3.03	0.02	−50.67	11.0	62.60	45.85	3328	−18.62	0.00	−296.97
14	7.7	72.68	63.89	440	−2.16	0.03	−28.62	11.0	48.25	34.33	2581	−14.42	0.01	−178.28
15	7.8	57.92	48.73	331	−1.49	0.05	−15.76	11.0	37.41	26.79	2010	−11.20	0.01	−107.71
16	7.9	46.36	36.88	247	−0.96	0.07	−8.34	11.0	29.16	21.45	1569	−8.70	0.01	−65.27
17	8.0	37.24	26.60	183	−0.56	0.12	−4.12	11.0	22.85	17.23	1228	−6.75	0.02	−39.60
18	8.1	36.67	26.51	170	−0.35	0.14	−3.42	13.6	20.97	20.49	1161	−5.24	0.03	−35.26
19	8.1	29.82	19.76	130	−0.08	0.22	−1.57	13.7	17.04	16.65	933	−4.06	0.04	−22.40
20	8.2	24.30	14.30	102	0.13	0.32	−0.59	13.7	13.90	13.55	752	−3.11	0.06	−14.23
21	8.2	19.86	9.86	86	0.29	0.46	−0.13	13.8	11.37	11.05	611	−2.36	0.09	−9.04
22	8.2	16.26	10.08	80	0.43	0.61	0.03	13.8	9.32	9.02	500	−1.75	0.14	−5.71
23	8.2	13.33	10.57	80	0.53	0.74	0.02	13.9	7.67	7.37	413	−1.26	0.21	−3.59
24	8.3	10.95	10.93	84	0.62	0.83	−0.08	13.9	6.32	6.02	347	−0.86	0.32	−2.24
25	7.9	89.79	78.65	575	−3.14	0.02	−49.45	13.2	51.83	50.77	3371	−18.54	0.00	−304.69
26	8.0	72.44	61.82	442	−2.28	0.03	−28.85	13.60	41.50	40.96	2683	−14.59	0.01	−192.60
27	8.1	58.64	48.41	338	−1.61	0.04	−16.48	13.7	33.55	33.16	2146	−11.53	0.01	−122.88
28	8.1	47.67	37.59	257	−1.09	0.07	−9.10	13.8	27.26	26.94	1725	−9.13	0.01	−79.05
29	8.2	38.86	28.86	194	−0.68	0.11	−4.75	13.8	22.24	21.94	1392	−7.23	0.02	−51.12
30	8.2	31.79	21.79	146	−0.36	0.17	−2.25	13.9	18.23	17.93	1128	−5.72	0.03	−33.25
31	8.2	26.06	16.06	111	−0.10	0.26	−0.87	14.00	14.99	14.68	918	−4.51	0.04	−21.67

TABLE 3 (continued)

	1983							1985						
	PROFILE CHARACTERISTICS		STATISTICS*					PROFILE CHARACTERISTICS		STATISTICS				
CASE	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF
32	8.3	21.44	11.40	87	0.10	0.38	−0.17	14.10	12.38	12.05	751	−3.54	0.06	−14.16
33	8.3	17.67	9.50	75	0.27	0.53	0.14	14.1	10.25	9.91	617	−2.76	0.09	−9.25
34	8.4	14.61	9.90	72	0.40	0.69	0.22	14.2	8.52	8.17	511	−2.12	0.14	−6.03
35	8.4	12.11	10.40	74	0.50	0.82	0.16	14.2	7.10	6.74	428	−1.60	0.20	−3.93
36	8.5	10.06	10.78	79	0.59	0.91	0.04	14.3	5.94	5.57	363	−1.17	0.30	−2.54
37	8.1	71.45	61.35	483	−3.05	0.02	−34.68	13.9	40.95	40.65	3080	−18.96	0.00	−254.17
38	8.2	58.27	48.27	373	−2.25	0.04	−20.21	14.0	33.39	33.08	2488	−15.17	0.01	−165.57
39	8.3	47.77	37.73	286	−1.62	0.06	−11.47	14.1	27.40	27.06	2024	−12.20	0.01	−109.25
40	8.4	39.35	29.21	218	−1.13	0.09	−6.23	14.2	22.62	22.23	1657	−9.86	0.01	−72.84
41	8.5	32.59	22.31	164	−0.73	0.14	−3.12	14.2	18.76	18.34	1363	−7.99	0.02	−48.98
42	8.5	27.07	16.69	123	−0.42	0.22	−1.33	14.3	15.64	15.19	1127	−6.48	0.03	−33.17
43	8.5	22.55	12.12	94	−0.18	0.33	−0.34	14.4	13.21	12.63	937	−5.26	0.04	−22.61
44	8.5	18.84	9.44	74	0.03	0.47	0.16	14.4	11.01	10.53	783	−4.26	0.06	−15.48
45	8.5	15.77	9.46	65	0.19	0.64	0.36	14.4	9.29	8.87	657	−3.44	0.08	−10.63
46	8.5	13.24	9.50	64	0.32	0.81	0.38	14.6	7.87	7.55	556	−2.76	0.12	−7.32
47	8.5	11.14	10.03	67	0.43	0.95	0.31	14.6	6.69	6.44	474	−2.20	0.17	−5.05
48	8.5	9.40	10.43	73	0.52	1.04	0.18	14.7	5.71	5.52	408	−1.74	0.24	−3.48
49	8.5	56.69	46.32	411	−3.07	0.03	−24.74	14.2	31.91	31.48	2815	−19.38	0.01	−212.21
50	8.5	47.06	36.50	320	−2.32	0.05	−14.65	14.4	26.48	25.96	2321	−15.82	0.01	−143.97
51	8.5	39.23	28.55	249	−1.73	0.08	−8.45	14.5	22.14	21.61	1930	−13.02	0.01	−99.22
52	8.5	32.83	22.09	193	−1.26	0.12	−4.66	14.6	18.64	18.28	1616	−10.78	0.01	−69.29
53	8.5	27.58	16.83	148	−0.88	0.18	−2.36	14.7	15.79	15.54	1362	−8.97	0.02	−48.94
54	8.5	23.26	12.52	114	−0.58	0.26	−0.99	14.8	13.45	13.28	1155	−7.50	0.03	−34.92
55	8.5	19.69	9.17	89	−0.33	0.38	−0.21	14.8	11.51	11.40	985	−6.28	0.04	−25.11
56	8.5	16.73	9.27	72	−0.13	0.54	0.21	15.0	9.91	9.83	845	−5.27	0.05	−18.20
57	8.5	14.26	9.34	63	0.03	0.73	0.39	15.0	8.56	8.50	728	−4.43	0.07	−13.27
58	8.5	12.20	9.39	61	0.17	0.94	0.43	15.1	7.43	7.39	631	−3.72	0.10	−9.73
59	8.5	10.48	9.50	63	0.28	1.11	0.39	15.1	6.47	6.44	551	−3.12	0.13	−7.16
60	10.2	9.17	9.90	68	0.38	1.23	0.30	16.2	5.65	5.63	484	−2.61	0.17	−5.30
61	7.4	55.89	47.69	307	−1.39	0.05	−13.36	13.1	5.45	4.48	231	−0.77	0.41	−0.44
62	7.4	38.73	30.59	190	−0.66	0.12	−4.52	13.1	2.62	2.00	146	0.15	1.90	0.43
63	7.4	26.85	18.74	117	−0.15	0.27	−1.10	13.1	1.26	2.90	167	0.59	4.67	0.25
64	7.4	18.61	10.54	82	0.20	0.55	−0.04	13.1	0.61	3.36	191	0.80	4.97	0.02
65	7.4	12.90	9.69	78	0.45	0.87	0.08	13.1	0.29	3.59	204	0.91	4.41	−1.12

66	7.4	8.95	10.71	86	0.62	1.02	−0.13	13.1	0.14	3.70	211	0.95	4.06	−0.20
67	7.4	6.21	11.42	97	0.74	0.98	−0.43	13.1	0.07	3.75	214	0.98	3.88	−0.23
68	7.4	4.31	11.91	106	0.82	0.90	−0.70	13.1	0.03	3.78	216	0.99	3.80	−0.25
69	7.4	2.99	12.24	112	0.87	0.83	−0.92	13.1	0.02	3.79	216	1.00	3.76	−0.26
70	7.4	2.07	12.48	117	0.91	0.78	−1.09	13.1	0.01	3.79	217	1.00	3.74	−0.27
71	7.4	1.44	12.64	121	0.94	0.74	−1.22	13.1	0.00	3.80	217	1.00	3.73	−0.27
72	7.4	1.00	12.75	123	0.96	0.71	−1.31	13.1	0.00	3.80	217	1.00	3.72	−0.27
73	7.3	50.76	41.94	282	−1.34	0.06	−11.12	11.0	6.54	3.30	198	−0.88	0.43	−0.06
74	7.3	35.18	26.60	173	−0.62	0.14	−3.57	11.0	3.15	1.45	123	0.10	2.04	0.60
75	7.3	24.38	15.97	106	−0.12	0.32	−0.73	11.0	1.52	2.57	158	0.57	5.02	0.32
76	7.3	16.90	9.50	77	0.22	0.64	0.09	11.0	0.73	3.21	187	0.79	5.14	0.06
77	7.3	11.72	9.50	77	0.46	0.97	0.10	11.0	0.35	3.51	202	0.90	4.47	−0.10
78	7.3	8.12	10.58	87	0.63	1.07	−0.15	11.0	0.17	3.66	210	0.95	4.08	−0.19
79	7.3	5.64	11.32	98	0.74	1.00	−0.46	11.0	0.08	3.73	214	0.98	3.89	−0.23
80	7.3	3.91	11.84	106	0.82	0.90	−0.73	11.0	0.04	3.77	215	0.99	3.80	−0.25
81	7.3	2.71	12.20	113	0.88	0.83	−0.95	11.0	0.02	3.78	216	1.00	3.76	−0.26
82	7.3	1.88	12.45	118	0.91	0.77	−1.11	11.0	0.01	3.79	217	1.00	3.74	−0.26
83	7.3	1.31	12.62	121	0.94	0.74	−1.23	11.0	0.00	3.80	217	1.00	3.73	−0.27
84	7.3	0.91	12.73	123	0.96	0.71	−1.32	11.0	0.00	3.80	217	1.00	3.72	−0.27
85	7.3	56.54	48.06	323	−1.58	0.05	−14.92	11.0	10.55	6.61	439	−2.32	0.13	−4.17
86	7.3	40.04	31.76	205	−0.83	0.11	−5.44	11.0	5.60	3.49	206	−0.80	0.51	−0.14
87	7.3	28.36	20.20	128	−0.29	0.23	−1.50	11.0	2.97	1.78	145	0.02	1.91	0.44
88	7.4	20.11	12.01	85	0.09	0.47	−0.11	11.0	1.58	2.55	162	0.47	4.70	0.29
89	7.4	14.26	9.50	73	0.35	0.79	0.19	11.0	0.84	3.14	184	0.71	5.52	0.09
90	7.4	10.12	9.52	79	0.54	1.01	0.05	11.0	0.45	3.45	199	0.84	4.90	−0.06
91	7.4	7.18	10.51	90	0.68	1.03	−0.23	11.0	0.24	3.61	207	0.91	4.37	−0.16
92	7.4	5.09	11.21	100	0.77	0.96	−0.52	11.0	0.13	3.70	212	0.95	4.07	−0.21
93	7.4	3.62	11.72	108	0.84	0.88	−0.77	11.0	0.07	3.75	214	0.97	3.91	−0.24
94	7.4	2.57	12.08	113	0.88	0.81	−0.96	11.0	0.04	3.77	216	0.99	3.82	−0.25
95	7.4	1.82	12.34	118	0.92	0.77	−1.11	11.0	0.02	3.79	216	0.99	3.78	−0.26
96	7.4	1.30	12.53	121	0.94	0.73	−1.23	11.0	0.01	3.79	217	1.00	3.75	−0.26
97	7.4	55.89	47.69	307	−1.40	0.05	−13.35	14.0	12.04	11.72	665	−2.73	0.08	−10.91
98	7.4	38.73	30.59	190	−0.66	0.12	−4.51	14.3	7.13	6.75	400	−1.17	0.24	−3.31
99	7.4	26.85	18.74	117	−0.15	0.27	−1.09	14.5	4.30	3.85	275	−0.28	0.73	−1.04
100	7.4	18.61	10.54	82	0.20	0.56	−0.03	14.6	2.62	3.33	227	0.23	1.93	−0.39
101	7.4	12.90	9.69	77	0.45	0.88	0.90	14.8	1.62	3.57	214	0.53	3.73	−0.23
102	7.4	8.95	10.71	86	0.62	1.02	−0.13	14.9	1.01	3.69	212	0.71	4.74	−0.21
103	7.4	6.21	11.42	97	0.73	0.99	−0.42	15.0	0.64	3.75	213	0.82	4.74	−0.23
104	7.4	4.30	11.91	105	0.82	0.91	−0.70	15.1	0.40	3.77	215	0.89	4.47	−0.24
105	7.4	2.99	12.24	112	0.87	0.83	−0.92	15.2	0.26	3.79	216	0.93	4.23	−0.25
106	7.4	2.07	12.48	117	0.91	0.78	−1.09	15.2	0.17	3.79	216	0.95	4.06	−0.26
107	7.4	1.44	12.64	121	0.94	0.74	−1.22	15.3	0.11	3.80	217	0.97	3.94	−0.26
108	7.4	1.00	12.75	123	0.96	0.71	−1.31	15.3	0.07	3.80	217	0.98	3.87	−0.27
109	7.3	50.76	41.94	282	−1.34	0.06	−11.11	13.8	8.76	8.46	553	−2.83	0.11	−7.24

TABLE 3 (continued)

	1983							1985						
	PROFILE CHARACTERISTICS		STATISTICS*					PROFILE CHARACTERISTICS		STATISTICS				
CASE	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF	DEPTH** (m)	PEAK*** (mg/kg)	ME (mg/kg)	RMSE (%)	CRM	CD	EF
110	7.3	35.18	26.60	173	−0.63	0.14	−3.55	14.1	5.14	4.83	325	−1.23	0.34	−1.85
111	7.3	24.38	15.97	106	−0.13	0.33	−0.71	14.3	3.07	2.83	231	−0.32	1.09	−0.44
112	7.3	16.90	9.50	77	0.22	0.65	0.10	14.6	1.86	2.99	206	0.21	2.92	−0.14
113	7.3	11.72	9.50	76	0.46	0.98	0.11	14.8	1.14	3.39	204	0.52	5.04	−0.12
114	7.3	8.12	10.57	87	0.62	1.08	−0.14	14.9	0.71	3.59	208	0.70	5.49	−0.16
115	7.3	5.64	11.32	97	0.74	1.01	−0.45	15.1	0.45	3.69	211	0.81	5.06	−0.20
116	7.3	3.91	11.84	106	0.82	0.91	−0.72	15.2	0.28	3.74	213	0.88	4.61	−0.23
117	7.3	2.71	12.20	113	0.87	0.83	−0.94	15.3	0.18	3.77	215	0.92	4.30	−0.24
118	7.3	1.88	12.44	117	0.91	0.78	−1.11	16.1	0.12	3.78	216	0.95	4.10	−0.25
119	7.3	1.31	12.62	121	0.94	0.74	−1.23	16.3	0.08	3.79	216	0.97	3.97	−0.26
120	7.3	0.91	12.73	123	0.96	0.71	−1.32	16.4	0.05	3.80	217	0.98	3.89	−2.26

* If all predicted and observed values were the same, then the statistics would yield: ME = 0; RMSE = 0; CRM = 0; CD = 1.0; and EF = 1.0. NOTE: The parameter values used for each case are listed in Table 2.

** Depth to peak concentration.

*** Peak concentration.

TABLE 4

SUMMARY OF RANKED PRZM SIMULATIONS BASED UPON STATISTICS FOR 4201a

	1983						1985						1983/ 1985
CASE	ME	RMSE	CRM	CD	EF	AVERAGE	ME	RMSE	CRM	CD	EF	AVERAGE	TOTAL AVERAGE
Base	36	36	52	5	35	27	60	61	13	10	61	28	14
1	121	121	121	121	121	121	121	121	117	72	121	121	121
2	118	118	116	118	118	118	119	117	112	70	117	117	117
3	114	113	110	113	113	113	115	111	107	64	111	111	112
4	106	105	99	105	105	104	110	106	101	59	106	106	107
5	99	98	63	98	98	95	105	101	96	54	101	101	101
6	85	84	22	84	84	80	91	91	89	45	91	91	90
7	75	50	1	76	50	52	84	85	84	39	85	85	78
8	23	29	18	69	29	30	79	76	78	31	76	77	61
9	14	12	31	60	12	20	70	68	70	21	68	70	45
10	19	14	42	44	14	23	63	62	65	15	62	54	30
11	26	23	48	28	23	24	57	57	61	8	57	42	21
12	35	32	59	18	32	33	55	55	22	4	55	23	15
13	120	120	117	120	120	120	118	119	119	72	119	119	119
14	117	115	112	115	115	115	114	114	113	67	114	114	114
15	113	110	106	110	110	110	107	108	108	62	108	108	109
16	101	99	97	100	99	99	101	102	102	56	102	102	103
17	92	91	47	93	91	89	96	97	97	50	97	97	96
18	89	88	29	90	88	86	100	96	90	49	96	96	95
19	83	83	4	83	83	72	95	89	85	43	89	89	88
20	74	49	9	75	49	54	90	84	79	37	84	84	80
21	20	35	26	68	35	37	83	77	72	29	77	76	64
22	25	26	36	61	26	32	78	71	67	19	71	71	57
23	32	27	45	49	27	34	71	65	63	14	65	60	50
24	40	31	55	32	31	40	64	59	25	9	59	34	26
25	119	119	120	119	119	119	120	120	118	72	120	120	119
26	116	116	114	115	116	116	117	115	114	67	115	115	116
27	112	111	108	111	111	111	113	110	109	62	110	110	111
28	102	101	98	101	101	100	108	105	104	58	105	105	105
29	94	95	63	95	95	94	103	100	98	53	100	100	100
30	86	85	31	86	85	82	97	94	93	47	94	94	92
31	78	58	6	80	58	58	92	88	88	41	88	88	85
32	44	40	7	70	40	42	87	83	82	36	83	83	68
33	8	16	23	65	16	18	81	78	75	30	78	79	53
34	22	8	34	56	8	18	74	72	68	20	72	71	44
35	27	13	43	34	13	21	68	66	64	16	66	62	40
36	39	25	50	20	25	25	61	60	60	11	60	48	25
37	115	117	118	117	117	117	116	118	120	70	118	118	117
38	111	112	113	112	112	112	112	113	115	66	113	113	113
39	103	104	109	104	104	105	109	109	110	61	109	109	108
40	95	97	100	97	97	98	104	104	105	56	104	104	104
41	88	87	66	89	87	90	99	99	100	51	99	99	98
42	79	81	35	82	81	78	93	93	95	46	93	93	90
43	54	43	15	72	43	48	88	90	91	42	90	89	78
44	5	15	2	66	15	11	82	86	86	38	86	86	53
45	6	5	16	59	5	6	77	80	81	32	80	80	42
46	14	4	27	36	4	4	73	75	76	24	75	74	33
47	24	6	36	14	6	5	66	69	69	18	69	67	23
48	28	11	44	12	11	12	59	64	66	13	64	52	20
49	107	114	119	114	114	114	111	116	121	67	116	116	115
50	100	108	115	108	108	108	106	112	116	64	112	112	110
51	93	100	111	99	100	100	102	107	111	60	107	107	106

TABLE 4 (continued)

	1983						1985						1983/ 1985
CASE	ME	RMSE	CRM	CD	EF	AVERAGE	ME	RMSE	CRM	CD	EF	AVERAGE	TOTAL AVERAGE
52	87	94	101	94	94	97	98	103	106	55	103	103	102
53	80	86	81	85	86	91	94	98	103	51	98	98	98
54	64	64	49	79	64	68	89	95	99	47	95	94	89
55	1	41	28	70	41	35	85	92	94	44	92	91	69
56	2	9	11	64	9	8	80	87	92	40	87	87	52
57	3	3	3	50	3	3	76	82	87	35	82	82	41
58	4	1	14	15	1	1	72	79	83	28	79	78	35
59	7	2	24	24	2	2	65	73	80	23	73	73	27
60	21	7	33	42	7	13	62	70	73	17	70	68	36
61	108	107	104	107	107	107	56	54	17	6	54	21	73
62	96	93	59	91	93	92	3	3	3	25	3	2	50
63	81	68	12	78	68	65	7	6	12	110	6	10	27
64	30	30	19	63	30	31	13	9	20	115	9	15	10
65	17	22	39	27	22	17	20	13	30	106	13	20	8
66	36	36	52	5	35	27	25	20	38	99	20	27	13
67	45	45	67	7	45	46	31	27	43	92	27	35	36
68	50	52	72	23	52	51	36	34	47	88	33	41	47
69	57	60	78	31	60	61	41	41	50	85	40	50	63
70	62	66	83	39	66	67	46	46	54	82	46	59	69
71	68	73	88	46	73	74	49	49	55	79	48	62	77
72	72	78	93	53	78	83	53	51	55	77	50	66	86
73	104	103	102	102	103	103	11	10	26	5	10	3	60
74	90	90	54	88	90	87	1	1	2	75	1	5	47
75	76	56	8	74	56	57	5	4	11	116	4	9	21
76	9	21	21	58	21	21	10	8	18	119	8	13	7
77	11	18	41	11	18	10	17	12	29	107	12	19	4
78	34	39	57	16	39	38	22	19	35	101	19	25	19
79	43	47	69	1	47	45	27	26	42	94	26	33	33
80	49	55	74	22	55	53	32	32	47	89	32	39	47
81	56	62	80	32	62	62	37	39	50	86	38	46	62
82	61	70	86	41	70	70	43	45	53	83	44	56	69
83	67	76	91	48	76	78	48	48	55	80	48	61	81
84	71	80	95	55	80	85	51	50	55	78	50	65	87
85	110	109	107	109	109	109	67	67	71	22	67	69	94
86	98	96	75	96	96	96	16	16	19	3	16	4	56
87	84	82	25	81	82	76	2	2	1	27	2	1	30
88	52	33	5	67	33	41	4	5	8	111	5	8	11
89	11	10	30	37	10	9	9	7	15	121	7	12	1
90	16	24	46	3	24	14	15	11	24	114	11	18	6
91	29	42	62	10	42	38	21	17	31	105	17	23	17
92	41	48	70	13	48	47	26	22	36	100	22	30	30
93	47	57	76	26	57	55	30	29	41	95	29	36	46
94	53	63	82	35	63	63	34	33	46	90	33	40	57
95	59	71	87	43	71	71	39	38	49	87	38	47	67
96	65	74	92	50	74	77	43	44	52	84	44	54	75
97	108	106	105	106	106	106	86	81	74	33	81	81	97
98	96	92	61	91	92	92	69	63	59	12	63	52	84
99	81	67	13	77	66	64	54	56	6	2	56	17	36
100	30	28	17	62	28	29	12	52	5	34	52	11	9
101	17	20	38	25	20	15	18	28	10	81	28	14	4
102	36	34	51	8	34	26	23	23	16	112	23	26	12
103	45	44	65	4	44	43	29	25	23	113	24	32	27
104	50	51	71	20	51	49	35	30	28	108	30	37	42

TABLE 4 (continued)

	1983						1985						1983/ 1985
CASE	ME	RMSE	CRM	CD	EF	AVERAGE	ME	RMSE	CRM	CD	EF	AVERAGE	TOTAL AVERAGE
105	157	59	77	29	59	59	40	35	33	103	33	44	57
106	62	65	83	38	65	66	45	37	36	98	37	49	66
107	68	72	88	45	72	73	49	42	40	96	42	58	75
108	72	77	93	52	77	81	51	47	45	91	46	62	83
109	104	102	103	102	102	102	75	74	77	26	74	75	93
110	90	89	57	87	89	87	58	58	62	7	58	43	74
111	76	53	9	72	53	55	6	53	7	1	53	7	18
112	9	19	20	57	19	16	8	15	4	76	15	6	2
113	11	17	40	9	17	7	14	14	9	117	14	16	3
114	33	38	56	17	38	36	19	18	14	120	18	22	16
115	42	46	68	2	46	44	24	21	21	118	21	28	23
116	48	54	73	19	54	50	28	24	27	109	24	31	36
117	55	61	79	29	61	60	33	31	32	104	31	37	53
118	60	69	85	39	69	69	37	36	34	102	36	45	65
119	66	75	90	46	75	75	42	40	39	97	40	51	69
120	70	79	95	53	79	84	47	43	43	93	42	56	82

NOTE: The parameter values for each case are listed in Table 2.

1985 (99) has the same hydrodynamic dispersion coefficient as the base case; the decay rate was slightly less; (5) The highest ranked (average) case for 1983 for 4201a (24) ranks only 37 for 1985; the highest ranked (average) case for 1985 for 4201a (74) is ranked 116 for 1983.

DISCUSSION AND CONCLUSIONS

The PRZM simulations undertaken for this study were designed to illustrate some of the nuances associated with dynamic-conceptual, multiparameter solute transport models. The interpretations of the 1985 simulations for 4201a are generally very similar to those described for 1983, although the model performance is much worse. If the 1983 simulations are used for calibration and the 1985 simulations are used for validation, or vice versa, then one must conclude that PRZM has not been calibrated for 4201a and that the model certainly cannot be described as validated. The results are still poor when the 1983 and 1985 simulations are both used for calibration. It is unreasonable, based upon the 120 simulations reported here, to suggest that either PRZM or the data base used as input to the model is appropriate for making long-term leaching predictions for EDB, or any other chemical, under conditions in Hawaii. As stated in the second part of this multipart paper (Loague et al. 1989*b*), PRZM was not designed to simulate pesticide movement over the extended depths included in this study; thus, the poor performance of the model is not surprizing. Problems associated with the model and the data sets, as well as suggestions for improvement, were described earlier (Loague et al. 1989*a*,*b*).

The conflicting results for the alternative model performance measures shown in this part of the paper illustrate the need for multicriteria evaluation procedures. The model performance results from any one statistical criterion or graphical display are not sufficient to pronounce a model's validation even if estabished levels of confidence were available. Taken independently, each method of evaluation can be limited by stringent assumptions. If even one assumption is violated, then sole

TABLE 5

SUMMARY OF RANKED PRZM SIMULATIONS BASED UPON EDB CONCENTRATION PROFILE CHARACTERISTICS FOR 4201a

	1983			1985			
CASE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	TOTAL AVERAGE
Base	60	13	24	88	74	91	54
1	56	121	113	37	121	84	115
2	53	118	110	50	118	100	118
3	47	114	101	50	114	93	113
4	47	106	94	50	110	87	106
5	47	99	90	54	104	84	102
6	47	85	80	1	95	43	63
7	39	74	58	1	90	41	38
8	39	59	40	1	82	35	20
9	39	33	22	1	75	32	9
10	9	19	8	1	36	12	3
11	9	1	2	1	14	5	1
12	1	16	4	1	5	3	1
13	58	120	115	1	120	61	103
14	58	117	112	1	117	59	99
15	56	111	105	1	113	56	96
16	53	100	94	1	108	53	84
17	47	92	84	1	103	49	75
18	39	91	77	55	99	80	90
19	39	84	69	57	94	75	81
20	9	75	30	57	89	73	42
21	9	60	20	60	83	71	35
22	9	34	14	70	77	69	25
23	9	21	10	65	69	67	22
24	1	2	1	65	19	37	5
25	53	119	111	50	119	101	121
26	47	116	102	55	116	103	117
27	39	113	93	57	112	101	113
28	39	102	87	60	106	96	107
29	9	95	48	60	101	89	76
30	9	86	38	65	96	89	67
31	9	78	33	69	91	87	60
32	1	71	22	72	86	84	48
33	1	43	16	72	79	75	35
34	6	27	12	76	71	74	30
35	6	10	3	76	31	52	10
36	19	6	7	81	15	43	8
37	39	115	98	65	115	112	118
38	9	112	66	69	111	112	104
39	1	103	48	72	107	111	93
40	6	97	47	76	102	110	90
41	19	87	53	76	98	107	95
42	19	81	43	81	92	106	85
43	19	72	36	85	87	105	78
44	19	51	21	85	81	96	57
45	19	30	17	89	76	95	50
46	19	20	13	92	70	91	44
47	19	4	6	92	25	58	16
48	19	9	8	97	12	53	15
49	19	110	76	76	109	116	112

TABLE 5 (continued)

	1983			1985			
CASE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	TOTAL AVERAGE
50	19	101	65	85	105	120	108
51	19	96	61	89	100	118	105
52	19	88	54	92	97	118	100
53	19	82	44	97	93	120	97
54	19	73	37	99	88	117	88
55	19	58	27	99	84	114	78
56	19	36	18	105	78	114	73
57	19	24	14	105	72	109	63
58	19	11	10	108	43	75	29
59	19	3	5	108	22	63	17
60	121	12	81	119	11	63	81
61	60	107	105	37	9	17	61
62	60	93	94	37	7	15	49
63	60	79	84	37	20	21	46
64	60	47	54	37	30	29	25
65	60	17	27	37	38	31	13
66	60	13	24	37	46	35	14
67	60	28	34	37	53	39	19
68	60	39	41	37	58	42	25
69	60	45	51	37	61	45	37
70	60	53	58	37	64	47	46
71	60	61	66	37	66	48	53
72	60	67	74	37	68	50	66
73	94	104	119	1	23	8	67
74	94	89	116	1	2	1	57
75	94	76	108	1	18	7	54
76	94	37	78	1	27	10	32
77	94	7	44	1	37	13	12
78	94	22	62	1	44	16	23
79	94	31	71	1	50	19	34
80	94	41	82	1	56	21	42
81	94	49	88	1	60	25	52
82	94	55	91	1	63	27	59
83	94	64	99	1	65	28	67
84	94	69	102	1	67	30	73
85	94	109	121	1	80	34	89
86	94	98	118	1	10	4	61
87	94	83	113	1	4	2	54
88	60	63	69	1	17	6	20
89	60	24	30	1	26	9	6
90	60	5	19	1	33	11	4
91	60	26	32	1	41	14	7
92	60	35	38	1	7	18	11
93	60	44	48	1	54	20	17
94	60	52	57	1	57	23	24
95	60	57	64	1	59	24	32
96	60	66	73	1	62	26	38
97	60	107	105	69	85	80	108
98	60	93	94	81	32	55	85
99	60	79	84	89	1	39	63
100	60	47	54	92	6	45	38
101	60	17	27	99	16	57	28
102	60	13	24	103	24	62	30

TABLE 5 (continued)

	1983			1985			
CASE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	DEPTH-TO-PEAK CONCENTRATION	PEAK CONCENTRATION	AVERAGE	TOTAL AVERAGE
103	60	28	34	105	29	67	41
104	60	39	41	108	35	71	50
105	60	45	51	112	40	79	72
106	60	53	58	112	45	82	77
107	60	61	66	115	49	93	93
108	60	67	74	115	52	99	101
109	94	104	119	60	73	66	108
110	94	89	116	72	8	33	85
111	94	76	108	81	3	37	83
112	94	37	78	92	13	50	71
113	94	7	44	99	21	60	44
114	94	22	62	103	28	65	67
115	94	31	71	108	34	70	78
116	94	41	82	112	39	75	90
117	94	49	88	115	42	82	98
118	94	55	91	118	48	96	111
119	94	64	99	120	51	103	116
120	94	69	102	121	55	108	118

NOTE: The parameter values for each case are listed in Table 2.

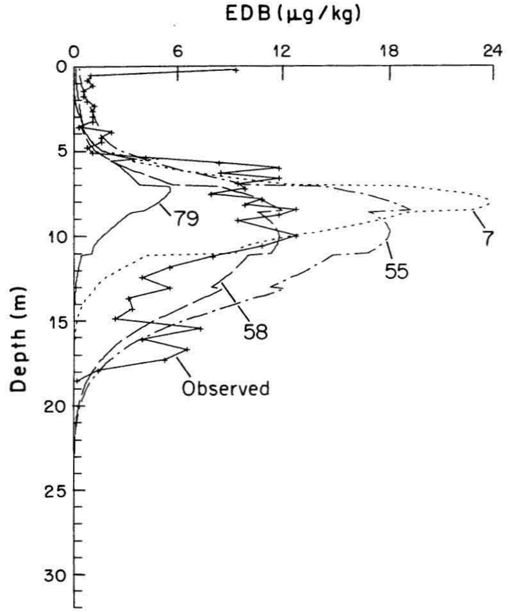

FIGURE 5. Observed versus predicted EDB concentration profiles for 4201a for 1983. The predicted profiles are those that ranked best based upon individual statistical criteria (Table 4).

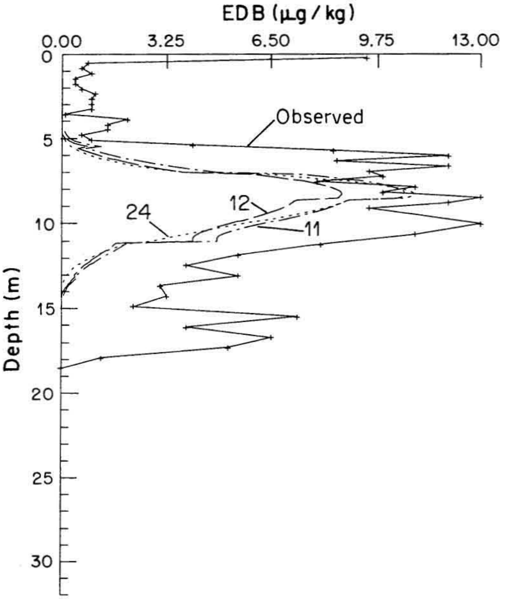

FIGURE 6. Observed versus predicted EDB concentration profiles for 4201a for 1983. The predicted profiles are those that ranked best based upon individual profile characteristics (Table 5).

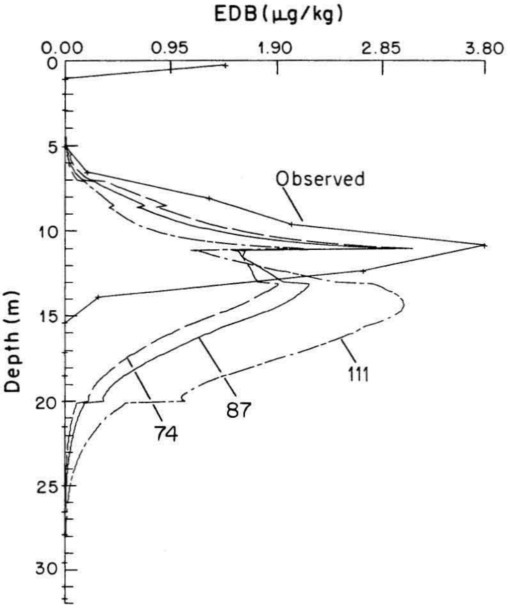

FIGURE 7. Observed versus predicted EDB concentration profiles for 4201a for 1985. The predicted profiles are those that ranked best based upon individual statistical criteria (Table 4).

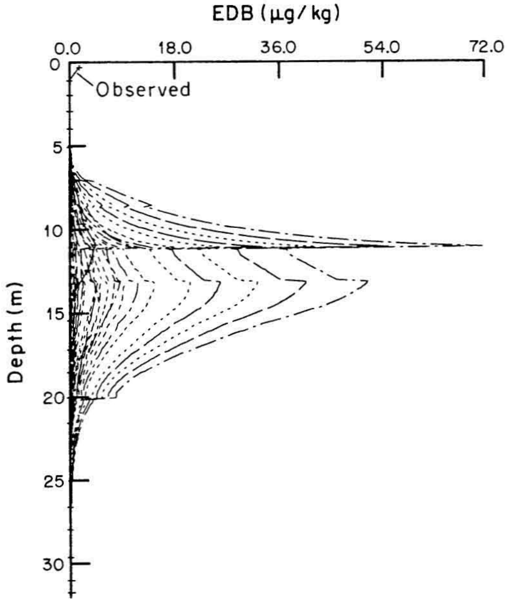

FIGURE 8. Observed versus predicted EDB concentration profiles for 4201a for 1985. The predicted profiles are those that ranked best based upon individual profile characteristics (Table 5). The case numbers for the predicted profiles are omitted.

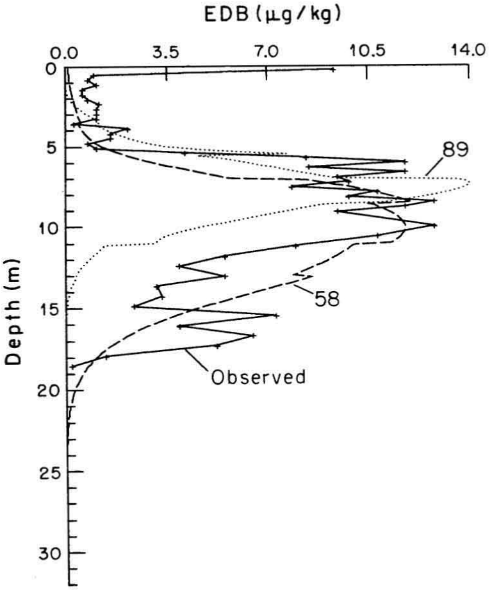

FIGURE 9. Observed versus predicted EDB concentration profiles for 4201a for 1983. The predicted profiles are those that ranked best based upon average statistical criteria (Table 4).

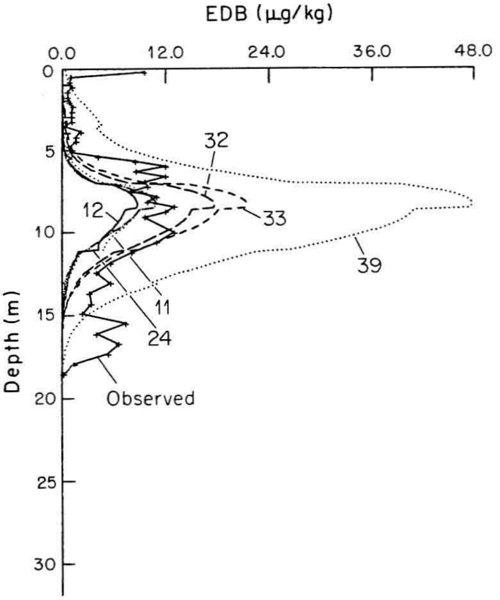

FIGURE 10. Observed versus predicted EDB concentration profiles for 4201a for 1983. The predicted profiles are those that ranked best based upon average profile characteristics (Table 5).

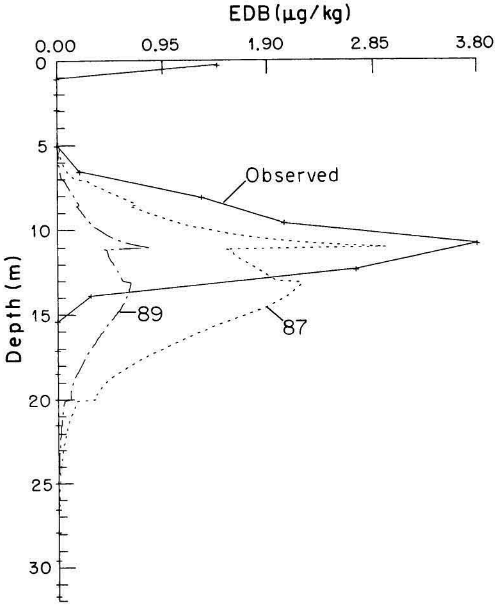

FIGURE 11. Observed versus predicted EDB concentration profiles for 4201a for 1985. The predicted profiles are those that ranked best based upon average statistical criteria (Table 4).

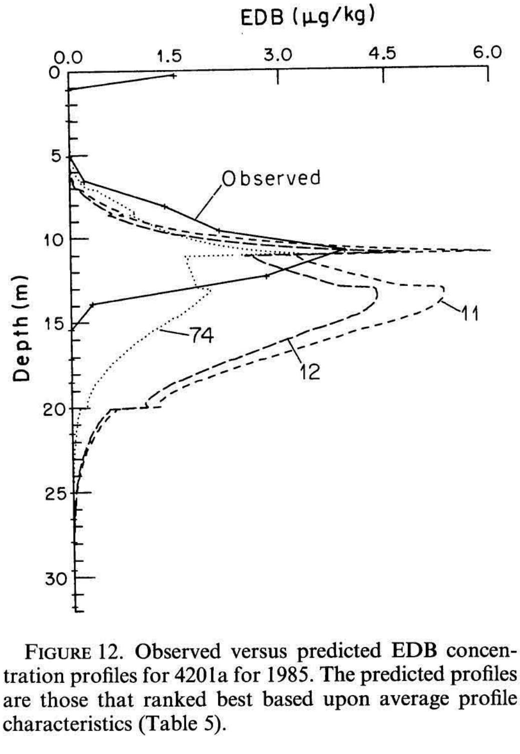

FIGURE 12. Observed versus predicted EDB concentration profiles for 4201a for 1985. The predicted profiles are those that ranked best based upon average profile characteristics (Table 5).

reliance on the method is suspect. A model should be considered validated only if a set of performance tests is met. In this effort results are combined, by ranking the results, from several tests to select the "best" simulation in a trial-and-error calibration. More effort in this area is needed to establish criteria and acceptable levels of performance for different objectives.

Generally, only a few of the parameters used in a dynamic simulation model, such as PRZM, are obtained directly from measurements at the locations where assessments of pesticide leaching are of interest. The missing information usually is estimated during the calibration of the model. Based on the initial results reported here, it appears that single concentration profiles from a single site at two different times are insufficient for a reliable model calibration and that several sites with profiles at various time intervals are needed. Chemical transformations complicate the model calibration and validation procedure tremendously. In fact, it may not be possible to validate certain pesticide leaching models for particular problems.

Improved field data sets are needed for model validation and comparison studies. The level of information for the model evaluation example discussed here is much more than is typical. Still, the data sets are far from perfect. Before specific model testing protocols can be established, we must first identify what information should be collected. We should not collect information only because it has been collected in the past. For each problem we must decide what should be measured, the number of measurements to make, where the selected measurements should be made, and how often. Of course, each data collection program and model validation problem is separate and ultimately a question of the utility for the information and a finite budget. Model evaluation can be as important as model selection. A model should be assumed suspect until it is proven correct. It would be very useful if a standardized model evaluation protocol is adopted. Once established, such procedures may be used to catalog model performance for different models and applications.

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