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Input Parameter and Model Resolution Effects on Predictions of Solute Transport

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ABSTRACT

Model predictions of solute transport using larger scale soil and climatic data sets may be useful for classifying mapping units based on their susceptibility to chemical leaching. However, model predictions based on input data sets with low spatial resolution may not accurately reflect transport processes occurring in situ. The goal of the current study was to compare several modeling approaches that might be applicable for classifying soil mapping units (1:24 000) according to their leaching potential to (i) model results based on detailed site-specific measurements and (ii) observed data collected at a field site (Borollic Calciorthid) in southwestern Montana. Data from a 2-yr field study of pentafluorobenzoic acid (PFBA), 2,6-difluorobenzoic acid (DFBA) and dicamba (3,6-dichloro-2-methoxybenzoic acid) transport in fallow and cropped systems under two water application levels were compared to simulations obtained using the Chemical Movement in Layered Soils (CMLS) and Leaching and Chemistry Estimation (LEACHM) models. The resolution of model input parameters was varied based on sources of data. In Case 1, model inputs were obtained primarily from detailed soil profile characterization and site-specific measurements of precipitation, irrigation, and pan evaporation. LEACHM predictions were also generated using estimated conductivity and retentivity functions from textural data obtained from the USDA-NRCS Soil Survey (SSURGO) database (Cases 2 and 3). CMLS predictions were generated using (i) detailed site-specific measurements (Case 1) and (ii) estimated volumetric water contents from textural data (SSURGO) and estimated daily precipitation and evapotranspiration (ET) from the Weather Generator (WGEN) and Montana Agricultural Potentials (MAPS) climate database (Cases 2 and 3). Comparison of observed and simulated mean solute travel times showed that (i) LEACHM and CMLS performed adequately with high-resolution model inputs, (ii) model performance declined when field conditions were conducive to preferential flow, (iii) estimated K_s values from regression equations based on textural data were problematic for generating adequate predictions using LEACHM, and (iv) CMLS predictions were less sensitive to data input resolution, due in part to the fact that CMLS provides an oversimplified description of transport processes.

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SUBSTANTIAL INTEREST in modeling the movement of chemicals through soils has developed because of concerns of groundwater contamination as a result of agrichemical application. Much of this interest is directed at mapping unit scale (e.g., 1:24 000) predictions. Approaches for predicting solute transport at mapping unit scales may involve coupling transport models with soil survey (SSURGO) databases, climate databases, and parameter estimation routines (e.g., pedotransfer functions, Wagenet et al., 1991) using Geographic Information Systems (GIS). However, uncertainties in data reliability, temporal and spatial variability of soil characteristics, and process simplification in deterministic models have often been considered formidable problems precluding the application of these tools for predicting solute transport at larger geographical scales.

Several field studies have been performed to evaluate the applicability of deterministic models such as LEACHM, CMLS, and PRZM for describing the transport of reactive and nonreactive solutes through soils (Comfort et al., 1993; Carsel et al., 1984; Pennel et al., 1990; Pearson et al., 1996a, b). Generally, these studies have relied on data input parameters that were carefully measured on-site and corresponded to the scale at which transport measurements were made (e.g., research plot scale). Coupling process-based solute transport models with larger-scale (e.g., 1:24 000) data sets in a GIS format represents a potential tool for screening or classifying soil mapping units for their susceptibility to chemical leaching below the root zone or into shallow aquifers (Zhang et al., 1990; Wilson et al., 1993). Recent attempts to develop screening indices to evaluate the susceptibility of groundwater resources to chemical contamination vary both in their consideration of site-specific soils and climate data and the methods used to predict potential for chemical movement out of the root zone. Screening indices such as those presented by Gustafson (1989) and Jury et al.

Abbreviations: PFBA, pentafluorobenzoic acid; DFBA, difluorobenzoic acid; LEACHM, Leaching and Chemistry Estimation; CMLS, Chemical Movement through Layered Soils; ET, evapotranspiration; MAPS, Montana Agricultural Potential System; WGEN, weather generator; GIS, Geographic Information Systems; BTCs, breakthrough curves; PET, potential evapotranspiration; AWC, available water-holding capacity.

(1987) rely primarily on pesticide properties describing sorption (K_{oc}) and persistence (half life, $t_{1/2}$). These methods are useful for classifying chemicals as leachers or nonleachers, the results of which generally correlate with the types of chemicals that are commonly found in well-water monitoring programs. However, these approaches do not consider site-specific soils or climate data that actually control the movement of chemicals through soils. Pickus and Hewitt (1992) described a pesticide-user management planning system (PUMPS) that integrates site-specific land use classification, groundwater depth, irrigation practices, pesticide characteristics, precipitation, ET, runoff and soils data. This information is coupled with a Leaching Pesticide Index model (Meeks and Dean, 1990; a one-dimensional advective–dispersive transport equation) to provide a value indicating the susceptibility of groundwater to pesticide contamination. Zhang et al. (1990) have also coupled soils and climate databases with a GIS system to produce predicted probabilities of exceeding Health Advisory Levels for specific chemicals in groundwater. Previous work by Wilson et al. (1993) outlined a method for coupling the USDA-NRCS State Soil Geographic Database (STATSGO, 1:250 000) and climatic information in the MAPS database with the one-dimensional CMLS (Nofziger and Hornsby, 1987) model to generate a frequency distribution of soil–climate polygons having predicted chemical movement to specific soil depths. More recently, Wilson et al. (1996) outlined methods for coupling the USDA-NRCS Soil Survey Geographic database (SSURGO, 1:24 000-scale) and the MAPS climate database with CMLS. The improved resolution of the Soil Survey database (SSURGO) resulted in a greater ability to identify mapping units with high potential for chemical movement below the root zone. The primary goal of the study by Wilson et al. (1996) was to evaluate the sensitivity of model predictions on data inputs obtained from different map scales and different attribute estimation routines. The current study uses some of the methods outlined by Wilson et al. (1993, 1996) to obtain solute transport model predictions based on data inputs obtained at mapping-unit scales. Our primary objective was to compare mapping unit-scale approaches for predicting chemical movement with observed field data collected at a site in southwestern Montana. We were specifically interested in (i) comparisons of observed data with those predicted using two transport models (CMLS and LEACHM) having different levels of process description, and (ii) comparisons of observed data with those predicted using model input parameters obtained from different scales of resolution.

MATERIALS AND METHODS

Field Experiments

In situ field column experiments were conducted on a Brocko silt loam (mixed, mesic Borollic Calciorthid) during 1991 and 1992. These experiments formed the basis of a more detailed comparison of observed and predicted (LEACHM) tracer and herbicide BTCs and profile water contents found in Pearson et al. (1996a, b). Briefly, PVC columns (0.2 m diam.) were hydraulically inserted to 1.2-m depth using cutting heads to minimize compaction. Columns were placed at different distances from a line source irrigation system to establish three water application levels (high, medium, and low). Half of the in situ columns (and surrounding area) were seeded to barley (*Hordeum vulgare* L. cv. Klages) to establish crop and fallow treatments at each water application level. All treatments were replicated either three (1992) or four (1991) times. Data and results presented here are limited to the high and medium water application levels. Solute BTCs at these water application levels were essentially complete at a depth of 0.66 m prior to the termination of the field experiment and more easily facilitate comparison of observed data with model results. The total water applied (irrigation plus precipitation) for high and medium water regimes was 52 and 42 cm during 1991, and 41 and 34 cm during 1992. Nonreactive tracers (PFBA in 1991 and 2,6-DFBA in 1992) were applied in 100 mL of solution per column at a rate of 112 kg ha^{-1} either 17 d (1991) or 48 d (1992) after seeding. In 1992, ^{14}C-labeled dicamba was applied with the 2,6-DFBA solutions at a rate of 0.26 kg ha^{-1}. Small (6 mm diam. by 80 mm length) porous ceramic cup lysimeters inserted horizontally into the column walls at 0.36, 0.66, and 0.96 cm were used to obtain soil solution samples 20 to 27 times throughout the growing season. Fluorobenzoates were analyzed using ion chromatography–conductivity detection (Pearson et al., 1992) and ^{14}C-dicamba was analyzed using scintillation. Selected samples were analyzed for dicamba and degradates using HPLC-radioisotope detection (Pearson et al., 1996b); in all cases, soluble ^{14}C was identified as dicamba. Concentrations of PFBA, 2,6-DFBA, and dicamba were plotted as functions of time for each lysimeter depth (0.36, 0.66, and 0.96 m) to establish breakthrough curves (BTCs) for each chemical. Moment analysis (Skopp, 1984) of complete BTCs (primarily the 0.36 and 0.66 m depths) was used to estimate the mean travel times (d) for center of solute mass for each water regime–cropping treatment.

Model Simulations

Modeling exercises were varied both with respect to model sophistication (CMLS vs. LEACHM) and the resolution of model input parameters (Table 1). Model input requirements and model assumptions are discussed in the original model documentation (Nofziger and Hornsby, 1987; Wagenet and Hutson, 1989), and are not repeated in detail here. Briefly, CMLS was developed primarily as a semiquantitative, deterministic model requiring only a minimal set of soil and climatic input parameters. The primary assumptions of CMLS include (i) water flow occurs in only one direction, driven by the water-holding capacity of individual soil layers, (ii) no solute dispersion, and (iii) input daily ET values may be met from any soil layer provided the water content in that layer (θ_z) is > -1500 kPa. LEACHM was developed to serve as a more exhaustive deterministic model with correspondingly greater input requirements. Primary assumptions include: (i) water flow according to the Richards equation with solute dispersion (convective–dispersion equation), and (ii) depth- and time-dependent root growth, water use (transpiration) and evaporation. Predicted solute BTCs obtained using LEACHM with Case 1 input parameters (mechanistic model with detailed site-specific measurements) represent a best case scenario for model performance. The intensity (or resolution) of input parameters required to generate model predictions at this scale (research field plot) is not realistic for larger geographic applications, such as at USDA NRCS mapping unit scales (1: 24 000). Consequently, additional modeling approaches, encompassing a range in model sophistication and parameter

Table 1. Outline of model simulations (CMLS and LEACHM) using various sets of input data† for evaluating mapping unit-scale predictions of solute transport.

Data input resolution		
Case 1	Case 2	Case 3
LEACHM		
SOIL: Detailed profile characterization, Campbell equation coefficients, ρ_b, K_s, OC, texture.	SOIL: Retention function parameters calculated from SSURGO mapping unit textural values and LEACHMRETPRED.	SOIL: Retention function parameters calculated from SSURGO mapping unit textural values and Rawls and Brakensiek (1989).
CLIMATIC: Precipitation, pan evap. and irrigation measured on site.	CLIMATIC: Precipitation, pan evap. and irrigation measured on site.	CLIMATIC: Precipitation, pan evap. and irrigation measured on site.
CMLS		
SOIL: Detailed profile characterization, ρ_b, θ_{sat}, θ_{-10kPa}, $\theta_{-1500kPa}$, OC.	SOIL: SSURGO Database, Rawls and Brakensiek (1989).	SOIL: SSURGO database, Rawls and Brakensiek (1989).
CLIMATIC: Precipitation and irrigation measured on site, actual daily ET from LEACHM Case 1.	CLIMATIC: MAPS Database and WGEN used to calculate 15 weather years. Actual ET estimated with Palmer drought model. Measured irrigation data overlaid on each weather year.	CLIMATIC: MAPS database and WGEN used to calculate 15 weather years. Actual ET estimated with Palmer drought model. Estimated irrigation events typical of regional cereal cropping systems.

† SSURGO = USDA-NRCS Soil Survey Geographic database (1:24 000). MAPS = Montana Agricultural Potentials (MAPS) climate database (Nielsen et al., 1990). WGEN = Weather Generator computer program (Richardson and Wright, 1984). ρ_b = Soil bulk density. θ_{sat}, θ_{-10kPa}, $\theta_{-1500kPa}$ = Volumetric water contents at saturation, −10 kPa, −1500 kPa. OC = Organic C.

estimation routines, were evaluated for comparison to the observed field data sets (Table 1).

LEACHM: Case 1

Independent measures or estimates of model input requirements were obtained as part of a previous study (Pearson et al., 1996a, b) and included dates of chemical application, planting, precipitation or irrigation events, a detailed soil profile characterization (Table 2) including soil bulk density, soil water retention, saturated hydraulic conductivity (K_s), soil organic C, soil texture, sorption coefficient for dicamba (K_{oc} = 0) and the principal degradate, 3,6-dichlorosalicylic acid (DCSA, K_{oc} = 504 L kg^{-1}) and degradation half-lives for dicamba and DCSA (dicamba = 13.5 d, DCSA = 40 d). Half-lives ($t_{1/2}$) for soil depths >0.3 m were estimated using a modified exponential decay function as outlined by Jury et al. (1987):

$$t_{1/2} = t_{1/2}(\text{surface})e^{\gamma(Z-L)} \quad [1]$$

where γ is a depth constant (1.5 m^{-1}), Z is soil depth (m), and L is depth (m) of the surface layer.

Daily precipitation, pan evaporation, and irrigation data were obtained throughout the field season for both 1991 and 1992 (data not shown, available from corresponding author upon request). Crop cover factors were estimated at 0.95 for this site, and the physiological maturity, as defined by LEACHM, was assumed to correspond to the booting stage, which occurred 58 d (1991) or 70 d (1992) after seeding. Minilysimeters (Lascano and van Bavel, 1986) were used to measure bare soil evaporation over two independent wetting–drying cycles (five replications per cycle) to determine an evaporation pan factor (0.6) for this site. Plant uptake of PFBA, DFBA, and dicamba was not allowed in the model simulations.

Model-predicted concentrations of soil solution PFBA, 2,6-DFBA and dicamba (mg L^{-1}) at 0.36 and 0.66 m depth as a function of time were written to a separate file, where moment analysis was used to obtain predicted mean travel times (d) for each water regime–cropping treatment.

LEACHM: Case 2

All inputs remained identical to Case 1 with the exception of soil physical properties necessary to estimate the soil–water retention function, and soil organic C content. Soils data for the Brocko silt loam mapping unit (1:24 000) corresponding to our field site were obtained from the USDA NRCS Soil Survey Geographic (SSURGO) database (Table 3). Although site-specific measurements of soil retention and hydraulic properties were obtained for six soil depth increments, only two soil layers are listed in the SSURGO database. This is consistent with the deep, uniform loess parent material from which the Brocko series has formed.

Bulk density and percent clay were determined from the midpoints of the ranges specified for each soil layer. Percent sand was computed from the average percentages of soil passing through No. 10 and 200 soil sieves, respectively (Wilson et al., 1993, 1996), and percent silt was determined by difference. Surface organic C content was determined from the midpoint of the range specified for organic matter multiplied by 0.5; organic C content of the second layer was determined using a regression expression relating organic C to soil depth developed from the Montana Soil Pedon Database (Jersey and Nielsen,

Table 2. Selected soil physical properties for the Brocko silt loam determined from detailed soil profile characterization.

Soil depth	Bulk density	Organic matter	Sand	Silt	Clay	AEV†	BCAM†	K_s
m	Mg m^{-3}	g kg^{-1}				kPa		mm d^{-1}
0.00–0.06	1.23	15.0	240	560	200	−1.65 (0.311)‡	4.64 (0.227)	124 (7.91)
0.06–0.14	1.29					−4.63 (0.655)	3.87 (0.192)	
0.14–0.30	1.22	11.7	180	620	200	−2.70 (0.270)	4.37 (0.130)	377 (94.0)
0.30–0.60	1.25	4.0	220	670	110	−9.72 (1.98)	1.65 (0.157)	825 (96.6)
0.60–0.80	1.31	1.3	270	650	80	−9.60 (1.69)	1.63 (0.134)	585 (229)
0.80–1.12	1.32					−6.55 (0.688)	1.83 (0.077)	

† AEV and BCAM determined by fitting the equation h = AEV (θv/θsat)$^{-BCAM}$ to soil water release data using nonlinear regression (θ_v determined at h values of 2.0, 5.0, 10.0, 20.0, 30.0, 50.0, 75.0, and 100 kPa).
‡ Standard errors in parentheses.

Table 3. Soil physical properties for the Brocko silt loam obtained from the USDA SCS (SSURGO) database and estimated values of θ(h) and saturated hydraulic conductivity (K_s).

Layer	Bulk density	Organic matter	Sand	Silt	Clay	θ_{sat}	θ_{-10kPa}†	$\theta_{-1500kPa}$†	K_s†
m	Mg m^{-3}	g kg^{-1}							mm d^{-1}
0–0.18	1.2	20	200	660	140	0.55	0.45	0.13	179
0.18–1.5	1.3	7	200	660	140	0.51	0.41	0.11	112

† θ_{-10kPa}, $\theta_{-1500kPa}$, and K_s predicted from Rawls and Brakensiek (1989).

1992; Wilson et al., 1993, 1996). Estimated soil physical properties for each layer were used to calculate saturated hydraulic conductivity (K_s) using regression equations developed by Rawls and Brakensiek (1989). Soil water retention based on particle-size distribution and the corresponding AEV and BCAM parameters of the Campbell (1974) equation were calculated using regression expressions contained in the LEACHM RETPRED subroutine.

LEACHM: Case 3

This model run used the same inputs as Case 1 with the exception of soil physical properties necessary to estimate the soil water retention function. As in Case 2, organic C, bulk density, and textural data were obtained from the SSURGO database for each soil layer (2). These data were then used in regression expressions developed by Rawls and Brakensiek (1989) to estimate K_s, AEV, and BCAM for direct input to LEACHM. Consequently, Cases 2 and 3 differ only in the method used to estimate soil water retention coefficients, both methods representing possible options for predicting soil–water retention characteristics from mapping unit (1:24 000 scale) soils data.

CMLS: Case 1

Soil properties required by CMLS include bulk density, organic C, and volumetric water contents (θ) at 0 (saturation), −10 and −1500 kPa matric potentials. Detailed soil profile characterization data were used as input to CMLS to correspond with Case 1 of the LEACHM simulations.

Precipitation and irrigation data (amounts and dates) were used as measured at the field site for both 1991 and 1992. CMLS requires actual daily ET rather than pan evaporation measurements of potential ET. In the absence of site-specific measured values of daily ET, estimates from Case 1 of the LEACHM simulation were used. LEACHM predictions (Case 1 inputs) of volumetric water content and bare soil evaporation were based on a detailed profile characterization and were in good agreement with measured values for both the 1991 and 1992 field seasons (Pearson et al., 1996a, b). Consequently, LEACHM predictions are considered to provide an accurate estimate of daily ET values.

Because CMLS assumes that the chemical pulse is of infinitely small thickness (i.e., no dispersion), the predicted time for a chemical to reach a given depth (e.g., 0.36 and 0.66 m) was assumed to correspond to the mean travel time (d) of a solute BTC obtained using moment analysis (Skopp, 1984).

CMLS: Case 2

Soil properties (bulk density, texture, and surface organic C) were obtained from the SSURGO database for each (2) soil layer and used to calculate necessary inputs for CMLS. As described in more detail in Wilson et al. (1993, 1996), soil textural data were used to estimate volumetric water contents at saturation, −10 and −1500 kPa using regression expressions obtained from Rawls and Brakensiek (1989). Organic C in subsurface horizons (only one additional layer for the Brocko silt loam) was calculated based on a regression expression relating OC as a function of soil depth developed from the Montana Soil Pedon Database (Jersey and Nielsen, 1992; Wilson et al., 1993, 1996).

Weather attributes (daily PET and daily precipitation) specific to this field site were obtained using the MAPS database (Nielsen et al., 1990) and the WGEN (Richardson and Wright, 1984). WGEN was used to predict 15 yr of daily precipitation based on long-term climate records and mean monthly values from the MAPS cell corresponding to the field site (Wilson et al., 1996). Solar radiation was used to estimate daily potential evapotranspiration (PET) values based on a solar thermal unit model developed by Caprio (1971). Actual ET was then calculated from daily PET values using the Palmer (1965) drought index model that requires estimates of available water-holding capacity (AWC) obtained from the SSURGO database for each soil layer. Daily precipitation and ET values were written to an input file required to run CMLS. Irrigation data (amount and date) measured during the field study were combined with each of the 15 different weather years, to obtain 15 different CMLS runs for each water regime for 1991 and 1992. These simulations are compared to only the crop treatments since the daily ET values computed with the Palmer model are intended to simulate ET in the presence of plants.

CMLS: Case 3

In the previous case, actual irrigation data for 1991 and 1992 was superimposed on predicted daily precipitation and ET. An additional run was performed using a generic irrigation schedule based on typical cereal production practices in this region. Two irrigation events (10 cm each on 1 and 20 July) were superimposed on each of the 15 weather years. The methods employed in this modeling run correspond very closely to what might be used to simulate transport based on soil mapping unit (1:24 000) and climate (MAPS and WGEN) databases, in the absence of detailed soil profile characterization and on-site measurements of pan evaporation, precipitation, or irrigation.

RESULTS AND DISCUSSION

Observed Solute Breakthrough Curves

Complete solute BTCs were observed for PFBA (1991), 2,6-DFBA (1992) and dicamba (1992) at 0.36 and 0.66 m for both the high and medium water application levels (see examples in Fig. 1). Pearson et al. (1996a, b) calculated percent solute recoveries over all depths and water application–crop treatment combinations, which ranged from 63 to 120% for PFBA (1991), from 94 to 150% for 2,6-DFBA (1992) and from 42 to 117% (some degradation to CO_2 during transport) for dicamba (1992). As expected, mean travel times (d) for all solutes increased with increasing soil depth (Tables 4–6). Differences in mean travel times between high and medium water applications were observed only under fallow con-

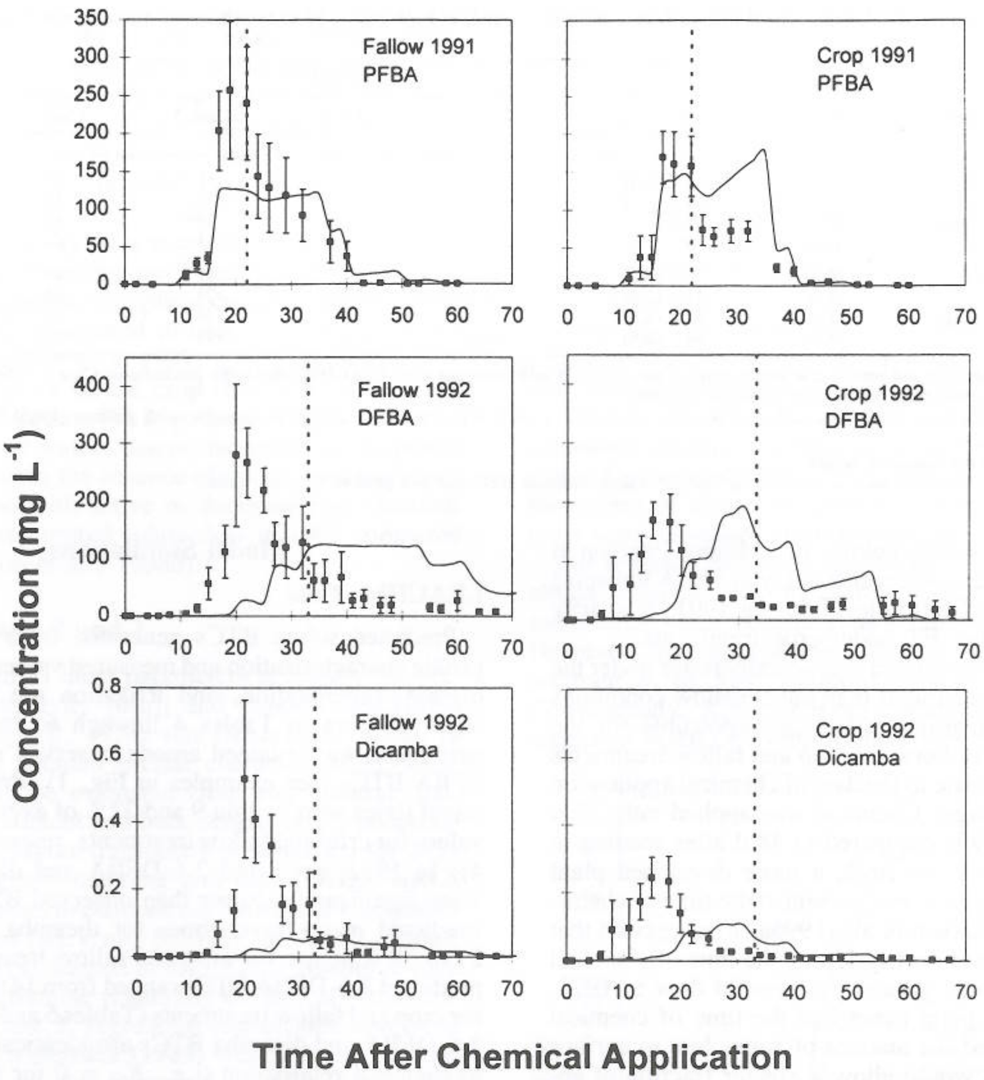

Fig. 1. Observed (■) and predicted (–) [LEACHM, Case 1 input data] solute breakthrough curves at 0.36 m for the medium water application level. Predicted centers of mass from CMLS, Case 1 input data are shown as dashed vertical lines. Error bars on observed data represent standard errors of three (1992) or four (1991) replications.

ditions; mean travel times for high and medium moisture regimes were similar under crop conditions. This may be due to increases in preferential flow paths caused by active and decaying root channels (Gish and Jury, 1983; Zins et al., 1991; Meek et al., 1992). In 1991, crop treatments resulted in delayed solute movement, espe-

Table 4. Observed and predicted mean travel times (d) of PFBA (1991) at 0.36 and 0.66 m depth under various water application-crop treatments.

Treatment	Water	Depth	Observed	LEACHM† Case 1	LEACHM† Case 2	LEACHM† Case 3	CMLS‡ Case 1	CMLS‡ Case 2
		m	d					
Fallow	High	0.36	14.2 (0.7)§	21.5	28	27	15	–
		0.66	26.1 (1.9)	32.3	45*	48*¶	39	–
	Medium	0.36	23.1 (1.6)	27.0	36	38	22	–
		0.66	42.2 (2.9)	43.8	46*	>60¶	40	–
Crop	High	0.36	24.3 (2.2)	22.5	29	28	15	15 (0)
		0.66	37.8 (1.2)	36.2	47*	49*	40	32 (1.6)
	Medium	0.36	24.0 (0.2)	26.0	36	33	22	16.9 (0.8)
		0.66	39.5 (1.0)	45.5	44	>60	49	39.2 (0.4)

† LEACHM Case 1 = detailed soil profile characterization; Case 2 = SCS soils database with LEACHM retentivity predictions; Case 3 = SCS soils database with retentivity coefficients from Rawls and Brakensiek (1989).
‡ CMLS Case 1 = detailed soil profile characterization with LEACHM Case 1 ET; Case 2 = SCS soils database with Palmer (1965) ET, 15 predicted weather years.
§ Values in parentheses are standard errors.
¶ * values indicate BTC was truncated on descending limb, > values indicate BTC had not peaked by given time.

Table 5. Observed and predicted mean travel times (d) of 2,6-DFBA (1992) at 0.36 and 0.66 m depth under various water application-crop treatments.

Treatment	Water	Depth	Observed	LEACHM† Case 1	LEACHM† Case 2	LEACHM† Case 3	CMLS‡ Case 1	CMLS‡ Case 2
		m	d					
Fallow	High	0.36	23.0 (4.8)	37.5	45	43	26	–
		0.66	46.2 (3.7)	52.6	>73	>73	62	–
	Medium	0.36	29.4 (3.8)	44.0	62*	57*	33	–
		0.66	60*	>73	>73	>73	64	–
Crop	High	0.36	26.9 (2.6)	27.3	41	39	26	28.6 (0.8)
		0.66	43.4 (2.6)	51.0	>73	>73	62	56.8 (0.9)
	Medium	0.36	26.2 (3.8)	34.3	47	44	33	31.7 (1.1)
		0.66	44.7 (2.9)	56.4	>73	>73	>73	61.8 (0.9)

† LEACHM Case 1 = detailed soil profile characterization; Case 2 = SCS soils database with LEACHM retentivity predictions; Case 3 = SCS soils database with retentivity coefficients from Rawls and Brakensiek (1989).
‡ CMLS Case 1 = detailed soil profile characterization with LEACHM Case 1 ET; Case 2 = SCS soils database with Palmer (1965) ET, 15 predicted weather years.
§ Values in parentheses are standard errors.
¶ *values indicate BTC was truncated on descending limb, > values indicate BTC had not peaked by given time.

cially at the high water regime. In addition, Pearson et al. (1996a) showed considerable delay in PFBA transport at a low water application level during 1991, primarily as a result of higher ET under crop treatments.

In 1992, solute movement was actually faster under the majority of crop treatments than under fallow conditions (Tables 5–6). The primary factors responsible for the differential behavior between crop and fallow treatments in 1991 vs. 1992 relate to the date of chemical application relative to crop stage. Chemical was applied only 17 d after seeding in 1991 compared to 48 d after seeding in 1992. Consequently, in 1992, a more developed plant canopy and root system was present at the time of chemical application. Pearson et al. (1996a, b) suggested that (i) a more developed root system at the time of chemical application promoted greater preferential flow in 1992, and (ii) a greater plant canopy at the time of chemical application reduced the amount of water lost as surface evaporation. This would allow a greater fraction of applied water to move into the subsoil, some fraction of which would eventually move to depths >0.36 and 0.66 m (function of depth-dependent root water uptake). These hypotheses were corroborated with LEACHM predictions in 1992, which showed faster predicted transport of 2,6-DFBA in crop vs. fallow treatments (Table 5).

Model Simulations

LEACHM: Case 1

Predicted solute BTCs generated from detailed soil profile characterization and measured values of pan evaporation, precipitation, and irrigation are compared to observed data in Tables 4 through 6. In 1991, good agreement was obtained among observed and predicted PFBA BTCs (see examples in Fig. 1). Predicted mean travel times were within 9 and 22% of average observed values for crop and fallow treatments, respectively (Table 4). In 1992, predicted 2,6-DFBA and dicamba BTCs were significantly slower than observed BTCs (Fig. 1). Predicted mean travel times for dicamba ranged from 27 to 38% higher for crop and fallow treatments, while predicted 2,6-DFBA BTCs ranged from 14 to 34% higher for crop and fallow treatments (Tables 5 and 6). Predicted 2,6-DFBA and dicamba BTCs are identical with respect to chemical retardation (i.e., $K_{oc} = 0$ for both solutes). However, dicamba is subject to degradation during transport. Degradation has a greater effect on the descending limb of solute BTCs that results in shorter mean travel times for dicamba compared to 2,6-DFBA.

Several factors may be responsible for the greater disagreement among observed and predicted BTCs in

Table 6. Observed and predicted mean travel times (d) of dicamba (1992) at 0.36 and 0.66 m depth under various water application-crop treatments.

Treatment	Water	Depth	Observed	LEACHM† Case 1	LEACHM† Case 2	LEACHM† Case 3	CMLS‡ Case 1	CMLS‡ Case 2
		m	d					
Fallow	High	0.36	21.4 (4.5)	31.9	41	38	26	–
		0.66	43.6 (4.0)	49.9	>73	>73	62	–
	Medium	0.36	25.9 (1.9)	39.1	44	43	33	–
		0.66	58*	>73	>73	>73	64	–
Crop	High	0.36	21.0 (1.0	24.2	38	34	26	28.6 (0.5)
		0.66	41.4 (3.5)	48.6	>73	>73	62	56.8 (0.9)
	Medium	0.36	20.5 (2.8)	30.6	44	43	33	31.7 (1.1)
		0.66	43.0 (3.9)	54.4	>73	>73	>73	61.8 (0.9)

† LEACHM Case 1 = detailed soil profile characterization; Case 2 = SCS soils database with LEACHM retentivity predictions; Case 3 = SCS soils database with retentivity coefficients from Rawls and Brakensiek (1989).
‡ CMLS Case 1 = detailed soil profile characterization with LEACHM Case 1 ET; Case 2 = SCS soils database with Palmer (1965) ET, 15 predicted weather years.
§ Values in parentheses are standard errors.
¶ * values indicate BTC was truncated on descending limb, > values indicate BTC had not peaked by given time.

1992 compared to 1991 (Pearson et al., 1996b). First, volumetric water contents were significantly higher immediately following chemical application in 1992 as a result of two irrigation events between 0 to 5 d of chemical application (Pearson et al., 1996b). Second, in situ columns used in 1992 had not been recently disturbed by surface tillage, and may have contained greater macroporosity as a result of biopore formation and aggregation (Hamblin and Tennant, 1981; Hamblin, 1982). Finally, chemical application occurred 48 d after seeding in 1992, compared to only 17 d after seeding in 1991. Consequently, in 1992, a well-developed root system was in place on the crop treatments at the time of chemical application. We hypothesized that a combination of higher soil water content, increased development of macroporosity in the absence of tillage, and macroporosity associated with active or decaying root channels caused more preferential solute flow in 1992 compared to 1991 (Pearson et al., 1996b).

LEACHM: Cases 2 and 3

LEACHM requires input parameters necessary for predicting soil retentivity [θ(h)] and conductivity [K(h)] functions (Campbell, 1974; van Genuchten, 1980). In the absence of detailed profile characterization, these coefficients may be estimated from soil textural data, organic matter content and bulk density (e.g., pedotransfer functions). Solute transport was simulated for 1991 and 1992 using soil mapping unit data (USDA NRCS SSURGO database) to estimate coefficients of Campbell's (1974) equations (AEV and BCAM). In Case 2, regression expressions contained in the LEACHM source code were used to determine retentivity coefficients from textural data. In Case 3, regression expressions developed by Rawls and Brakensiek (1989) were used to estimate the coefficients of the Campbell equation (AEV and BCAM) from textural data and porosity. Although these parameter estimation routines are quite similar (LEACHM uses a similar set of equations developed by Rawls and Brakensiek (1989), but first generates θ(h) data for fitting a modified version of Campbell's equation), we wanted to compare results using both approaches as either might be considered a feasible alternative for estimating solute transport from soil mapping unit data.

Predicted mean travel times using estimated retentivity and conductivity functions were considerably greater than observed values and LEACHM predictions based on detailed profile characterization (Case 1) (Tables 4–6). Previous comparisons among observed and predicted PFBA (1991) BTCs based on detailed soil profile characterization demonstrated that LEACHM predictions were within 9 to 22% of observed mean travel times (Pearson et al., 1996a). Consequently, with appropriately measured input parameters, LEACHM adequately described solute movement in 1991. Discrepancies between measured and estimated conductivity functions were identified as the primary cause for differences in predicted mean travel times among LEACHM Case 1 and Cases 2 to 3.

The estimated retentivity functions for Cases 2 and 3 input assumptions were in general agreement with measured θ(h) and the fitted function based on measured data (Fig. 2). However, the estimated $K(\theta)$ function deviated substantially from $K(\theta)$ generated with measured data, primarily at lower profile depths (>0.3 m) (Fig. 3). Saturated hydraulic conductivity (K_s) plays a major role in the shape of this function. Calculated $K(\theta)$ functions (Cases 2 and 3) were based on K_s estimated from textural data (Table 3). Estimated and measured K_s values were close for the surface layer (0–0.18 m), and the resultant $K(\theta)$ functions were also similar (Fig. 3). The estimated K_s of 112 mm d^{-1} for the subsurface layer was significantly lower than the majority of measured values for subsurface horizons (Table 2) and resulted in estimated conductivity functions that greatly underestimated K at water contents >0.3. This explains the slower movement of solutes in cases where conductivity functions were estimated from textural data.

For research plot scale applications, it is important to obtain independently measured values of K_s or K at some other water content(s) as a function of soil depth. However, for mapping unit scale applications, obtaining accurate K_s or $K(\theta)$ values is generally not possible. Consequently, $K(\theta)$, or more commonly, K_s, must be estimated based on available data (texture and bulk den-

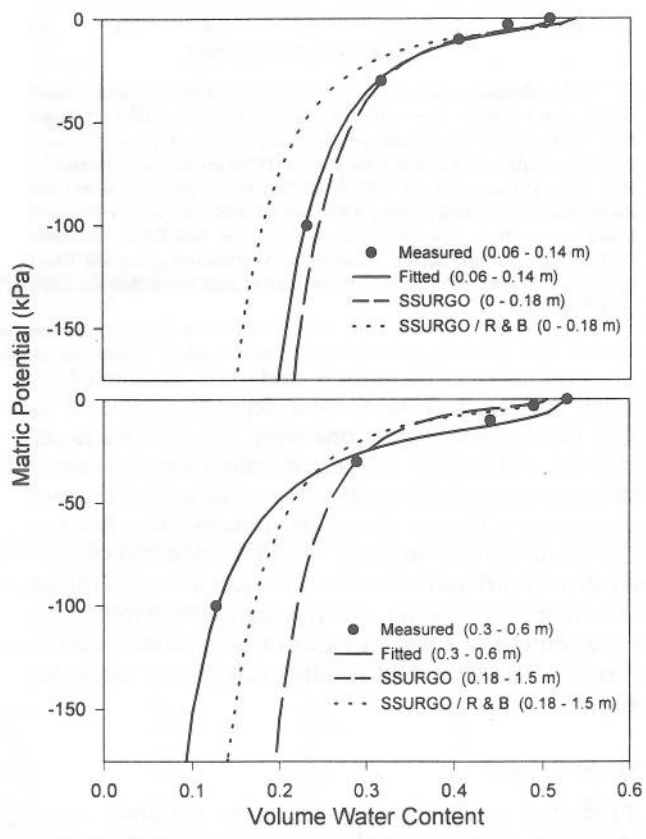

Fig. 2. Measured and predicted soil water retention relationships for surface and subsoil layers. Curves were generated by LEACHM using different input data, including (*i*) AEV and BCAM calculated by fitting Campbell's (1974) equation to measured data (Fitted), (*ii*) particle size distribution from the SSURGO database (SSURGO), and (*iii*) AEV and BCAM estimated using SSURGO particle size data plus equations in Rawls and Brakensiek (1989) (SSURGO/R&B).

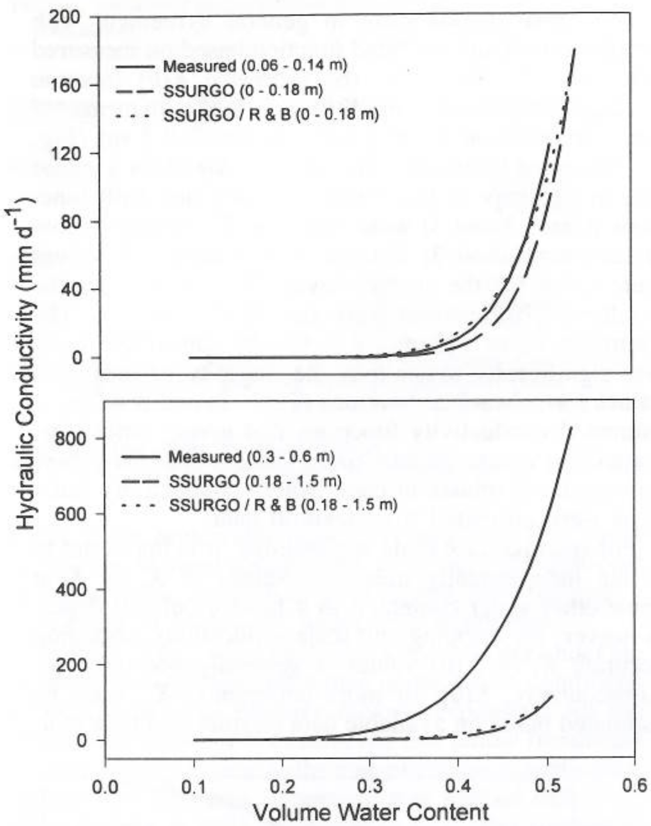

Fig. 3. Soil hydraulic conductivity relationships for surface and subsoil layers. Curves were generated by LEACHM using different input data, including (*i*) K_s measured on intact soil cores plus AEV and BCAM calculated by fitting Campbell's (1974) equation to measured θ(h) data (Measured), (*ii*) K_s from SSURGO particle sizes and Rawls and Brakensiek (1989), AEV and BCAM internally estimated based on particle size distribution from the SSURGO database (SSURGO), and (*iii*) K_s, AEV and BCAM estimated using SSURGO particle size data plus equations in Rawls and Brakensiek (1989) (SSURGO/R&B).

sity). Even though the current study was conducted on a rather uniform soil (deep loess deposit), estimated K_s values for subsurface horizons were significantly lower than measured values. Measured values were obtained with intact cores that retained structural and/or biopore characteristics. Greater deviations in subsurface horizon K relative to surface horizons would be expected considering that (i) surface horizons are subject to annual tillage that disrupts aggregation, and (ii) regression expressions for predicting K_s are largely based on textural characteristics rather than structural features that impart macroporosity.

CMLS: Case 1

Predicted mean travel times were obtained using CMLS with detailed profile characterization data (bulk density, values at saturation, −10 and −1500 kPa) and LEACHM-estimated ET values as input parameters. Mean travel times predicted for 1991 using CMLS were generally very similar to LEACHM (Case 1) predictions and observed values. In 1991, CMLS (Case 1) predictions averaged only 3.5% higher than observed, compared to LEACHM (Case 1) predictions that averaged between 9 and 22% higher. In 1992, CMLS (Case 1) predictions averaged 24% higher for 2,6-DFBA and 38% higher for dicamba. This compares to LEACHM (Case 1) predictions that averaged 24% higher for 2,6-DFBA and 32% higher for dicamba.

Although model resolution is quite different for CMLS and LEACHM, differences in model performance were slight given similar input parameter resolution (Case 1 inputs). Mean travel times predicted using CMLS tended to be higher than LEACHM predictions at the 0.66 m depth for the majority of water application–crop treatments, but were nearly identical at the 0.36 m depth. The water and chemical flow subroutines in LEACHM (based on the Richards equation with dispersion) are more sophisticated than flow calculations in CMLS (based on tipping-bucket with no dispersion). Furthermore, depth-dependent ET losses are essentially nonexistent in CMLS, where water can be extracted from the profile by roots at any depth and time provided θ_z is > -1500 kPa. Evapotranspiration in LEACHM is partitioned based on (i) potential surface evaporation, and (ii) potential transpiration that is based on a depth- and time-dependent root distribution function. Under the current conditions, LEACHM and CMLS provided similar estimates of mean travel times for both 1991 and 1992 despite these differences in model resolution.

CMLS: Case 2

CMLS simulations were also performed using soils data obtained from the USDA NRCS (SSURGO) database, coupled with weather and ET predictions (15 weather years) that correspond to a mapping unit scale (1:24 000) approach (Wilson et al., 1993, 1996). Results from this simulation are presented only for the crop treatments since the method of predicting actual ET (Palmer, 1965) was developed for vegetated surfaces. Mean travel times obtained using these input parameters were lower than those obtained using detailed soil profile characterization data (CMLS: Case 1), and were often closer to observed values (Tables 4–6). In fact, mean travel times for several treatments were closer to observed values than LEACHM predictions using carefully measured (Case 1) input parameters. It is ironic that improved agreement was obtained for several water application–depth combinations using a simpler model based on estimated soil physical and climatic characteristics (i.e., lower resolution input parameters). However, improved CMLS predictions using Case 2 inputs do not result from an improved description of chemical or physical processes operating in the soil profile. Rather, they are a direct result of differences between carefully measured and estimated input parameters, which only coincidentally improved model simulations. The primary factor identified that contributed to the lower mean travel times for Case 2 vs. Case 1 CMLS inputs relates to differences in input ET values. Estimated ET values using the Palmer (1965) drought model and available water-holding capacity of various soil layers (Wilson et al., 1993, 1996) were approximately 10 to 20% lower than ET values generated using LEACHM with carefully measured input parameters. We showed previously that LEACHM-predicted soil water contents and surface evaporation were in good agreement with observed data for both 1991 and 1992 (Pearson et al., 1996a, b). Consequently, estimated ET values based on the Palmer model and values of AWC from the SSURGO soils database underestimated ET for conditions specific to this study. Lower ET values used for CMLS Case 2 inputs contributed to shorter predicted mean travel times (i.e., greater water flow), which in 1992, resulted in improved agreement between observed and simulated values.

CMLS: Case 3

As demonstrated with Case 2 CMLS input parameters, reasonable agreement was obtained between observed and predicted mean travel times. However, these predictions still relied on actual irrigation events overlaid on 15 different estimated weather years. For mapping unit applications, detailed irrigation data (exact quantities and time of application) will not be available, yet it is important to account for irrigation provided it is a dominant crop production practice for a given mapping unit. For the Brocko silt loam mapping unit, estimates of sprinkler irrigation amounts were obtained by evaluating typical crop production practices. Predicted mean travel times for a nonsorbing tracer obtained using these estimates averaged 29.8 $\pm$ 2.2 d at 0.36 m and >73 d at 0.66-m depth (compare to 1992 data, Tables 5–6). These values are in general agreement with CMLS predictions based on detailed irrigation inputs (Case 2), and under these condtions, suggest that generic irrigation estimates may be acceptable for mapping unit scale applications.

In the semiarid and arid regions common to the western USA, irrigation is a common production practice. Under these conditions, it is important to know how critical accurate daily precipitation estimates are in facilitating satisfactory model outcomes. Both CMLS Case 2 and Case 3 were evaluated using 15 different synthetic weather (daily precipitation and ET) years. The average precipitation amounts during the growing season are relatively low compared to applied irrigation (e.g., in our field study, <20% of total applied water). Consequently, mapping unit scale transport predictions under irrigated conditions are not nearly as sensitive to variations in daily precipitation. For example, the standard errors associated with predicted mean travel times over 15 different weather years were very low for all CMLS Case 2 and Case 3 predictions (generally in the range of 1–3% of mean values). For comparison, CMLS predictions of mean travel times under dryland conditions (no irrigation) showed that the depth of solute movement after one growing season ranged from 0.12 to 0.31 m over 15 different weather years with an average depth of 0.22 m and a standard error approaching 10%. Consequently, under dryland conditions, variations in yearly weather patterns are more critical. However, under irrigated conditions, the amount of precipitation occurring during the growing season probably does not justify laborious procedures to generate stochastic weather data.

SUMMARY

Simulated mean travel times for PFBA (1991) obtained using LEACHM and CMLS with high resolution input parameters (Case 1, detailed site measurements) compared well with observed data (within 3–20%). Despite detailed input parameters (Case 1), both models overestimated mean travel times for 2,6-DFBA and dicamba (1992) possibly because of field conditions conducive to preferential flow. LEACHM predictions based on NRCS soils data and estimated retentivity and conductivity functions (Cases 2 and 3) resulted in poorer agreement with observed data. Estimated K_s for the subsurface layer was significantly lower than observed values, which resulted in slower predicted water and solute movement. Mean travel times obtained using CMLS with estimated parameters from NRCS soils databases and MAPS/WGEN were in reasonable agreement with CMLS and LEACHM simulations based on more detailed Case 1 input parameters, and in some cases (1992) resulted in better agreement with observed data. Closer agreement to observed data was considered merely coincidental and due primarily to lower ET estimates using MAPS/WGEN and the Palmer model. Nevertheless, the fact that CMLS produced reasonable estimates of mean travel times based on mapping unit scale (1:24 000) input parameters suggests that this may be a reasonable approach for classifying the susceptibility of mapping units in terms of solute movement.

Questions concerning estimation of chemical transport at mapping unit scales have centered on (i) the accuracy and reliability of solute transport predictions based on mapping unit scale input parameters, and (ii) the appropriate models to complement the resolution of available input data. Conceptually, the application of CMLS vs. LEACHM for predicting solute movement at mapping-unit scales (e.g., 1:24 000) is quite different. CMLS is a simple estimation model that requires a minimum set of soils and weather data. Consequently, mapping unit predictions using CMLS require a minimal set of parameter estimation routines (mainly θ values at saturation, -10 and -1500 kPa) and some estimate of daily precipitation and actual ET. However, CMLS oversimplifies several important processes such as depth- and time-dependent ET, and hydrodynamic dispersion. The requirement to externally estimate actual daily ET is also inconvenient at best. Conversely, LEACHM is a fairly detailed deterministic model and requires a correspondingly greater number of input parameters. On one hand, data available at mapping unit scales may not support the use of a model with this level of process description and required input parameters. However, parameter estimation routines (e.g., pedotransfer functions; Wagenet et al., 1991) and ad hoc stochastic methods may be applied to determine effects of parameter estimation on model outcomes. For example, in the current study, estimation of K_s from textural data was problematic for obtaining reliable LEACHM predictions based on mapping unit scale input parameters. Knowledge of critical input parameters affecting model predictions can be used to direct and refine soil survey data collection and use. Optimally, predicting solute transport at mapping unit scales would combine a minimal set of the most pertinent water flow, solute partitioning, and solute transformation routines with possible provisions for preferential flow and capabilities to vary input parameters using an ad hoc or truly stochastic approach.

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