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MEMORANDUM

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SUBJECT: USE OF LEACHM MODEL, LEACHP VERSION TO PREDICT VOLATILIZATION COMPONENT OF A PESTICIDE LOST FROM A FIELD APPLICATION

Summary

LEACHP version of LEACHM model was used to predict the volatilization component of Telone® (1,3-dichloropropene [1,3-D]) using data from Knuteson et al. (1992). They measured a cumulative loss of 11.2 percent of the applied pesticide over eight days after application. Using pesticide, soil, and meteorological data from Knuteson et al. (1992) as input to LEACHP, resulted in predicted cumulative loss of 17.9 percent for the same period when the soil segment thickness was set at 5 mm. However, increase in modeled segment thickness increased the predicted losses for the same period. The fact that the cumulative volatilization is highly dependent on segment thickness creates uncertainty in the use of this model for predicting volatilization, despite the relatively close agreement achieved with the smallest segment size. The larger proportion of the predicted losses took place during early days from treatment, whereas the observed losses were larger during the latter part of the study period. This weakened the model utility. The concentration of 1,3-D in the top-most soil segment should correlate with the rate of volatilization loss. Thicker segment simulations that gave larger losses were expected to have larger concentrations in the top most layer. However, the model predictions were the opposite of this expectation. Similarly, higher moisture content in the top-most soil segment was expected to slow the loss of 1,3-D to air. Since the least volatilization loss occurred with the 5mm thick segment simulation, the soil moisture in the top-most segment in this simulation was expected to be the highest over the eight day period. The predicted soil moisture in 5 mm simulation for this period did not fully support this expectation. In the quasi-steady state conditions for days five to eight, the 5 mm simulation established the lowest moisture and lowest flux compared to simulations run with thicker segments. An analysis on the sensitivity of the model to changing the initial soil temperature conditions revealed that the model responses were minimal to the range tested. Because of these difficulties I conclude that the LEACHP version of the LEACHM model is not a suitable tool to predict the loss to air from soil application of a highly volatile pesticide like 1,3-D.

BACKGROUND

LEACHM model was developed over a period of years (the first manual released in 1997). It is a useful tool to model the movement of water and solutes in soils in relation to specific conditions of soil texture and climatic factors (Hutson and Wagenet, 1992). LEACHP version 4 of this model can predict the vertical movement (one dimensional) of a pesticide through soil, if the model parameters for pesticide are available. It can also predict the volatilization component of a pesticide. Troiano et al. (1993) used LEACHM model to give a physically based explanation for the differences in water movement between sprinkler and basin irrigation methods. They further showed that atrazine moved in water to different soil depths depending on soil properties and irrigation method. Spurlock et al. (2006) used LEACHM to assess the ground water contamination by pesticides in the Central Valley of California. They demonstrated that LEACHM could predict the movement of simazine and diuron through the root-zone of the soil types in these study areas reasonably well. The Department of Pesticide Regulation (DPR) has been intensively engaged in regulation of soil fumigants. A critical element in fumigant management is the rate of transfer from soil to air (flux). It would be beneficial for the program to be able to assess flux using simulation modeling. Towards that end, I undertook a comparison between modeled and measured flux values. The focus in this study was to estimate the volatilization component of 1,3-D using this model and compare it with the measured volatilization reported by Knuteson et al. (1992). With this model, I estimated (a) flux, (b) concentration of 1,3-D, and (c) moisture in soil. If these estimates are acceptable, it is intended to test the model predictions further with other studies. If the model predicts volatilization component of an applied pesticide with acceptable accuracy, then LEACHP may be another tool to estimate the portion of a pesticide that escapes to air after an application. Such a tool would assist in mitigating fumigant volatilization.

METHODS

LEACHP model (October 25, 2005 version) is designed to receive data from a study in the form of an input file (Table 1 and Appendix 1). The first part of the input file covered the study settings such as starting date, ending date, time interval, profile depth, and segment thickness. The next part consisted of information on the status of water movement. The input file next required information on the type of output files, summary files, and breakthrough files expected in the results. The next part was information on soil physical properties related to the field study, followed by crop data when relevant. The next group of input information required in the model was on initial profile chemical data on the chemicals used in the study and associated chemical properties including, transformation and degradation rate constants, and chemical application information. This is the place to input data on fumigant application point in the soil profile (which segment[s]), and application rate in to the input file. If there was any cultivation done, that information was inputted. Data on rain and rainwater composition accounted for all of the water coming in to the study field. The next set of input information was on weather data for a specified period that included the study period. Knuteson et al. (1992) measured most soil properties to a maximum depth of 90 cm (Appendix 1). Bulk density was measured to a depth of 60 cm. The soil temperature was measured at

2.5 cm, 10 cm, 30 cm, and at 50 cm respectively. These data were the initial conditions for that simulation. The model required specifying a soil segment thickness. A series of runs using thick (100 mm) to thin (5 mm) segments were done in order to test for this possible effect on model output. The segment thicknesses were 100, 75, 50, 25, 20, 10, and 5 mm. Model also required that the profile depth to be divisible by segment thickness. For segment thickness of 75 mm, a profile depth of 975 mm was used and in all other simulations the profile depth was 1000 mm.

Table 1: Some of the values used in the input file reported in Appendix 1 for 100 mm segment thickness simulation.

Input file property	Parameter	Details	Source
Soil Physical Properties	Depth clay, slit, Org. C, B.D*. , Ini. Mois** % % % 0-10 cm 28.7 39.5 0.55 1.33 0.114 10-20 cm 28.5 39.5 0.55 1.33 0.114 20-30 cm 25.5 45.7 0.24 1.44 0.209, continues up to depth 90-100 cm * Bulk Density (kg/dm^3), ** Initial Moisture Content (v/v)	Soil properties are measured up to 90 cm, Bulk density up to 60 cm, Soil ^{0}T at 2.5, 10, 30, 50 c.m. depths	Knuteson et al., 1992, Pg 60, Pg 64. Pg 67.
Initial Chem. Profile (What pesticide, placed where in the soil profile)	Soil Layer: 5, i.e. between 40-50 cm depth, (Note: this soil layer number will change with the changing segment thickness in other input files) Application rate mg/kg of dry soil	1,3-D: 94.45 (mg/kg) was placed in this segment of soil	Knuteson et al., 1992, Pg 14
Chemical Properties (of 1,3-D)	Solubility Vapor Density (VD) Link 1 (Yes) Uptake 0 (No) Koc, Alpha	2320 mg/dm^3 VD = 4540 mg/dm^3 Link 1 set to 100 No uptake =0 K_{OC} = 27.66 (l/kg), Alpha = 0.693 (a constant)	Knuteson et al., 1992, Pg. 14 VD Calculated using Vapor Pressure, Pg 14, LEACHM Manual LEACHM Manual
	Diffusion coefficients		LEACHM Manual
Transformation and Degradation Rate Constants (RC)	Rate Constant (RC) set to flag 0 Base T^0 20 ^{0}C Optimum T^0 35 ^{0}C Maximum T^0 50 ^{0}C To calculate Degradation Rate constant, the soil degradation half life value of 6.3 days was used based on Dugan et al. 2001.	Flag 0 means no transformation. 4.12, a factor by which RC changes per 10 ^{0}C increase in temperature Base temp. =20 ^{0}C Opti. temp. =35 ^{0}C Max temp. =50 ^{0}C Degradation Rate Constant for 1,3-D =0.11	Knuteson et al., 1992, Pg 64, Pg 65 LEACHM Manual LEACHM Manual
Number of water applications	1 (at least 1 required in the model)	1 mm (to keep it minimum since no water was applied in the study)	LEACHM Manual

RESULTS AND DISCUSSION

Table 2: shows flux measured in Knuteson et al. (1992). Given in Figure 1 is a plot of this field data for study sampling intervals.

Table 2: Aerodynamic flux and mass volatilized from Imperial Valley Study				
Actual time in February	**Cumulative hours from end of treatment**	**Interval**	**Flux of 1,3-D (mg/m2/hr)**	**Mass 1,3-D volatilized kg/6.07 ha**
19th-1200-1800 -day1	6	1	3.44	1.25
19th-1800-2400-day1	12	2	1.68	0.61
20th-0000-0600-day2	18	3	1.67	0.61
20th-0600-1200-day2	24	4	0.29	0.11
20th-1200-1800-day2	30	5	3.74	1.36
20th-1800-2400-day2	36	6	3.94	1.44
21st-0000-0600-day3	42	7	1.99	0.72
21st-0600-1200-day3	48	8	4.92	1.79
21st-1200-1800-day3	54	9	7.12	2.59
21st-1800-2400-day3	60	10	12.10	4.42
22nd-0000-0600-day4	66	11	3.56	1.30
22nd-0600-1200-day4	72	12	2.34	0.85
22nd-1200-1800-day4	78	13	7.07	2.75
22nd-1800-2400-day4	84	14	13.80	5.02
23rd-0000-0600-day5	90	15	3.33	1.21
23rd-0600-1800-day5	96	16	3.78	2.75
23rd/24th-1800-0600-day5	102	17	10.80	7.90
24th-0600-1800-day5	108	18	11.30	8.22
24th/25th-1800-0600-day5/day6	120	19	13.50	9.84
25th-0600-1800-day6	132	20	13.60	9.92
25th/26th-1800-0600-day6/day7	144	21	20.40	14.84
26th-0600-1800-day7	156	22	13.00	9.50
26th/27th-1800-0600-day7/day8	168	23	3.94	2.87
		total loss kg/6.07 ha		91.70
		total applied kg/6.07 ha		817.38
		Percent volatilized (91.70/817.38)*100 =		11.20

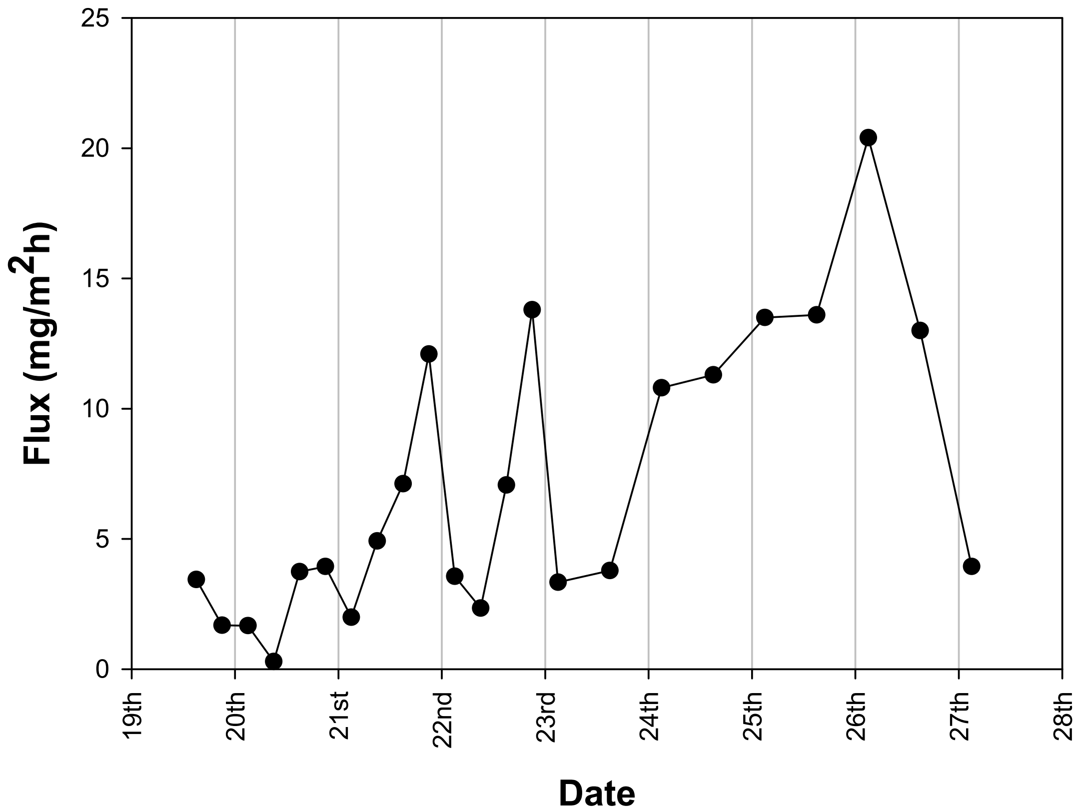


Figure 1. Flux profile for 1,3-dichloropropene for the Imperial Valley study. Study was conducted in Februrary, 1991.

From the data in Table 2, and Figure 1 it is evident that measured losses of 1,3-D during first few days were relatively smaller compared to the later days (five to seven) from application. The maximum flux was 20.4 mg/m^2-h, which occurred 6 days after application. Three peaks in the flux profile occurred during night time (Figure 1).

Figure 2: Cumulative volatilization loss (mg/m2) of 1,3-Dichloropropene from 100 mm, 25 mm, and 5 mm segment simulations

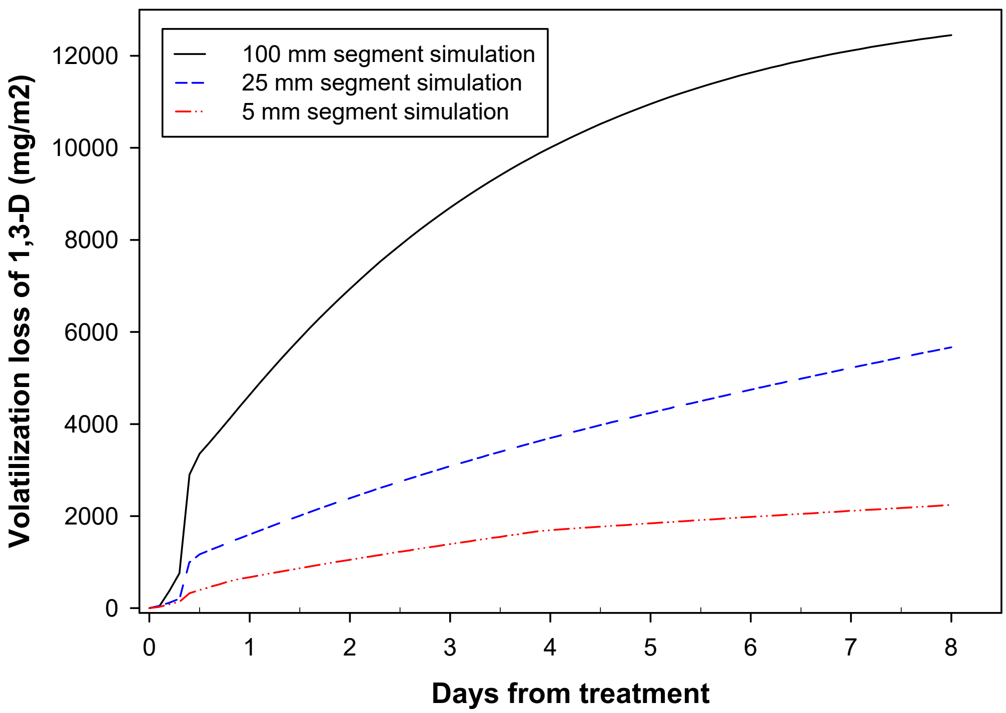


Figure 2 shows the predicted cumulative loss of 1,3-D over eight days from the end of application of this pesticide for three simulations. For clarity 75, 50, 20, and 10 mm segment simulations are omitted. It should be noted that the simulation started at the midnight of the first day as required by LEACHP. Hence, the comparisons will not refer to actual time lapses, but to relative time lapses. For example, the first six hour period from the beginning of simulation was midnight to 0600 hours in the morning, but in the actual study this was from noon to 1800 hours of the same day. The comparisons would be made for similar intervals of simulated vs. observed, which is another limitation of the model.

Table 3: Daily cumulative loss of 1,3-D due to volatilization, expressed as a percentage of initial amount applied from three simulations and from Imperial Valley study, and the average daily flux predicted for 5 mm segment simulation and the observed average daily flux from Imperial Valley study.

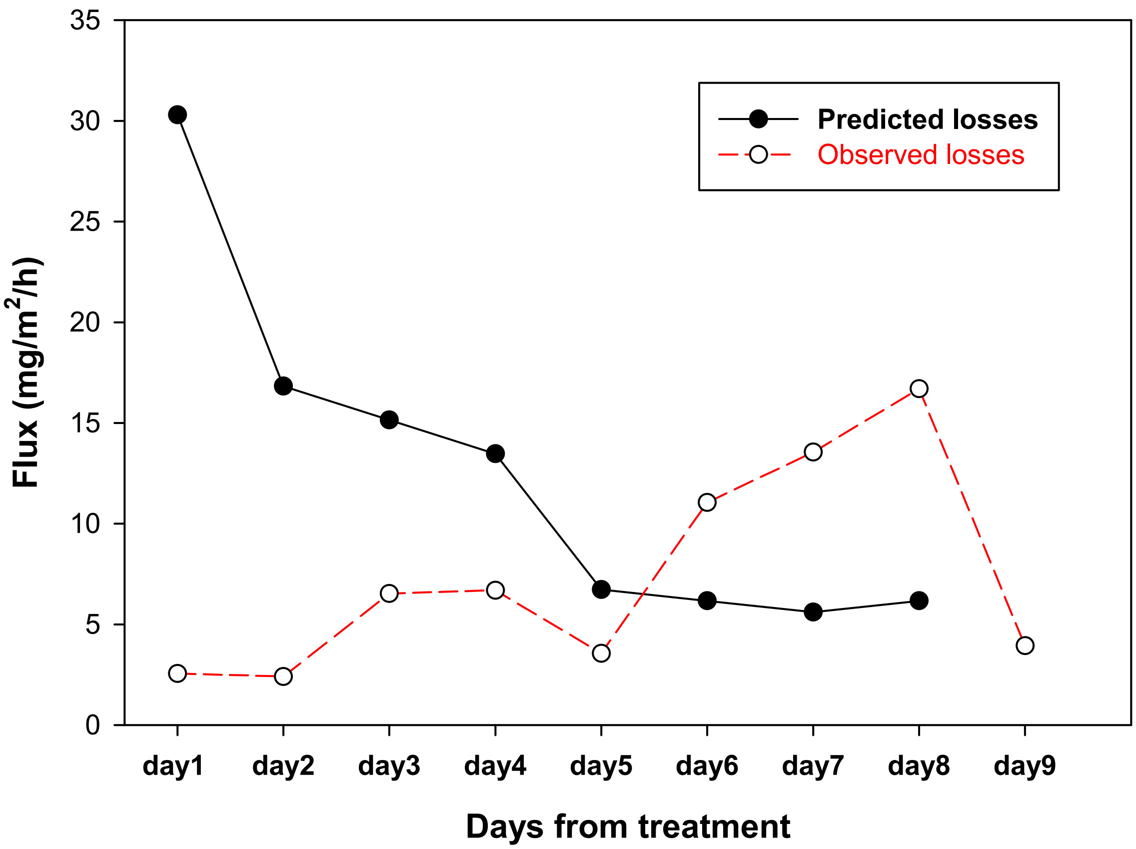
Percent Cumulative. Loss	**Day 1**	**Day 2**	**Day 3**	**Day 4**	**Day 5**	**Day 6**	**Day 7**	**Day 8**	**Day 9**
100 mm simulation	36.9	55.2	69.3	79.6	87.2	92.6	96.4	99.1	
25 mm simulation	12.8	19.0	24.5	29.4	33.8	38.7	41.5	45.1	
5mm simulation	5.4	8.4	11.1	13.5	14.7	15.8	16.8	17.9	
Imperial Valley Study Filed Obs.*.	0.2	0.7	1.8	3.0	3.5	5.5	7.9	10.9	11.2
Flux									
Average daily flux predicted in 5 mm simulation ($mg/m^2/h$)	30.30	16.83	15.15	13.47	6.73	6.17	5.61	6.17	
Average daily flux observed in Imperial Valley Study	2.56	2.41	6.53	6.69	3.56	11.05	11.55	16.7	3.94

*Note that in the Imperial Valley study observations for Day 1 and Day 9 were only 12 hours long.

The 8 day cumulative loss due to volatilization for 100 mm simulation was 99.1 percent of the total 1,3-D used. When degradation losses were added, total exceeded 100 percent. This 100 mm thick segment simulation carried a mass error of approximately 16 percent of the applied 1,3-D mass. The cumulative volatilization loss for 25 mm simulation was 45.1 percent, about 4 times the measured volatilization. These predicted values are too different from the measured values to be considered useful. For 5 mm segment simulation, the cumulative loss due to volatilization for the 8 day period was 17.9 percent of the total used. The two smaller segment thickness simulations had no mass error. Mass error was not included in estimation reported. A similar amount was lost due to degradation. Cumulative measured volatilization loss for the same period was 11.2 percent (Table 3). The 5 mm segment simulation predicted volatilization loss (17.9 percent) was relatively closer to field measured value of 11.2 percent.

The 9-day trend in daily average flux differed between predicted and measured values (Table 3-Flux, and Figure 3). Measured daily flux intermittently increased, whereas the modeled flux generally decreased. This response reduces the value of the model as an accurate predictor of 1,3-D loss.

Figure 3: Predicted 24 hour average flux for 5 mm segment simulation vs observed flux from Imperial Valley study of 1,3-D for 9 day period



The model predicted volatilization was measured in more detail. The interval of a day was divided to 10 equal parts, giving a period of 2.4 hours per division. There were high spikes in losses at the 0.4-day interval, for all three simulations (Figures 4a and 4b). One possible explanation is that the model assumes both evaporation and transpiration to start at 0.3 day (0720 hrs) and end 12 hours later at 0.8 day with a maximum at 0.55 day (1320 hours)(LEACHM manual, page 84). If this is the case, then this pattern should be repeated each day, at a decreasing intensity, since there will be lesser amount available for evaporation as cycles repeat. However, results show only one peak on the first day.

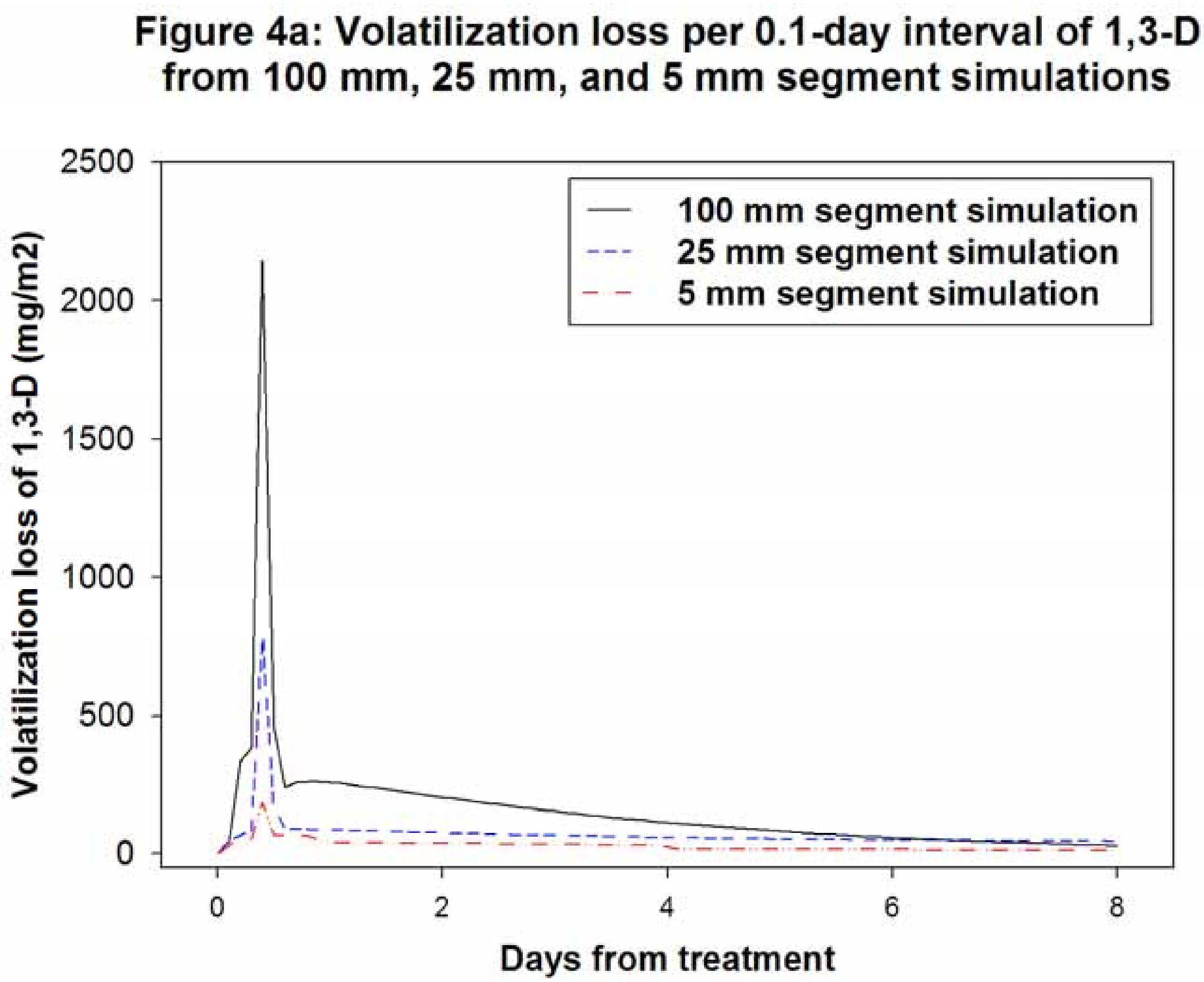
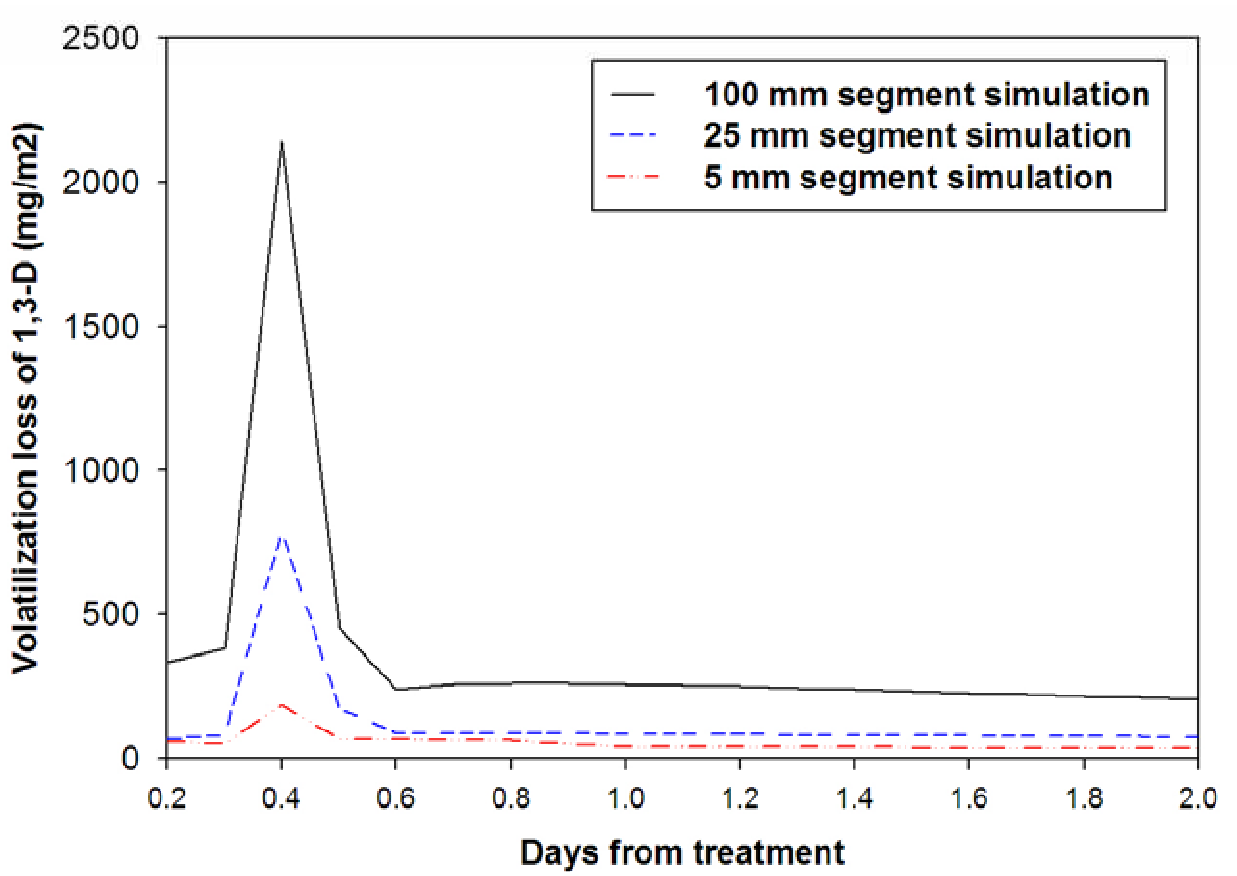


Figure 4a: Volatilization loss per 0.1-day interval of 1,3-D from 100 mm, 25 mm, and 5 mm segment simulations
Volatilization loss of 1,3-D (mg/m2)
2500
2000
1500
1000
500
0
100 mm segment simulation
25 mm segment simulation
5 mm segment simulation
0
2
4
6
8
Days from treatment

Figure 4b: Volatilization loss per 0.1-day interval of 1,3-D from 100 mm, 25 mm, and 5 mm segment simulations zoomed for 2 days



Thicker segment simulations such as 100 mm and 75 mm segments predicted larger losses relative to thinner ones (10 mm and 5 mm). Therefore, it is reasonable to expect the top-most segment of the thicker segments that is in contact with air to have a higher concentration of 1,3-D than the top segment of the thinner segment simulations. The sum file was set to yield the concentration of 1,3-D in the top segment to be similar to input file segment thickness. For example, in the 100 mm thick segment simulation input file, the first segment of the sum file also could be set to a 100 mm thick segment. This way one can obtain the concentration of 1,3-D in the top segment. Figure 5a shows the concentrations per day in the top segments from the sum files for 100 mm, 25 mm, and 5mm thick segment simulation. Figure 5b shows the concentrations when zoomed to 0.1 day intervals.

Figure 5a: 1,3-D concentration (mg/dm^3) in top bulk soil segment from 100 mm, 25 mm, and 5 mm segment simulations

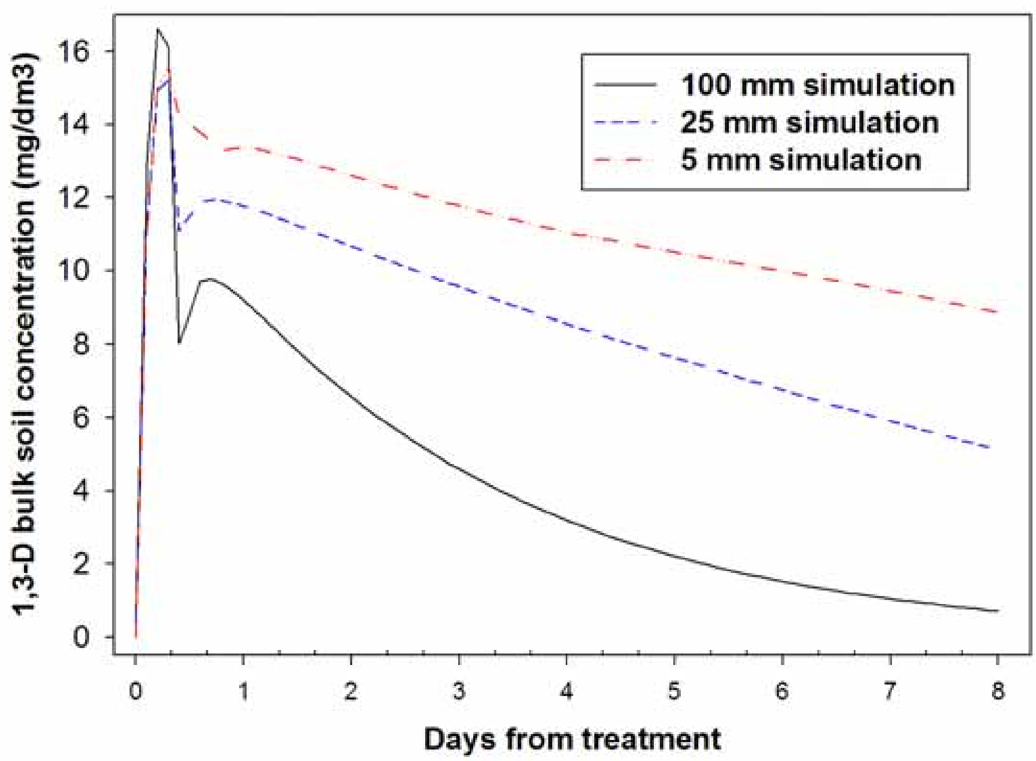
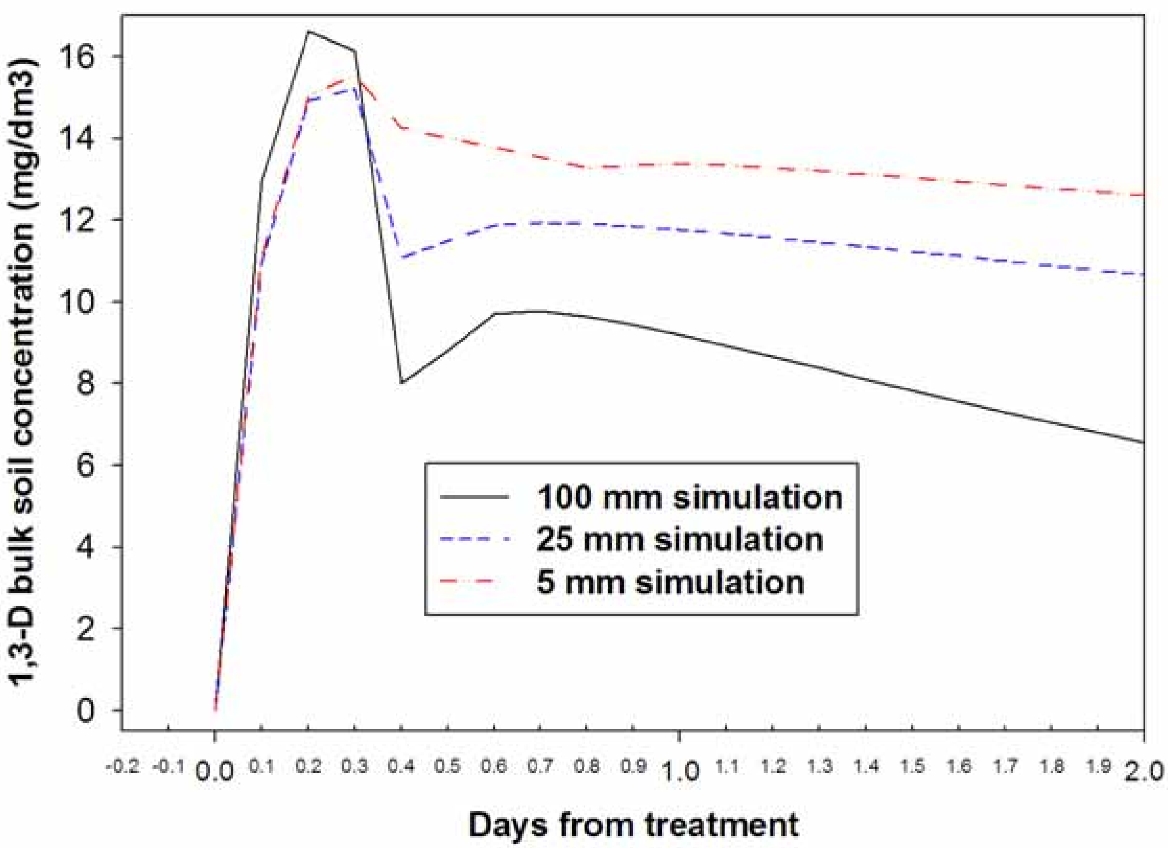


Figure 5b: 1,3-D concentration (mg/dm^3) per 0.1 day interval in top bulk soil segment from 100 mm, 25 mm, and 5 mm segment simulations zoomed to 2 days



The results in Figures 5a and Figure 5b should be looked in at two steps. In step 1, the thickest segment (100 mm) simulation carried the highest concentration of 1,3-D up to 0.3 day interval (Figure 5b). Step 1 prediction was consistent with the model-predicted flux for 100 mm segment simulation because the 100 mm segment simulation showed the highest flux. If step 1 was consistent for all simulations, then the next thick segment (25 mm) should have the next highest 1,3-D concentration, but it was not, and 5 mm segment carried slightly higher 1,3-D than 25 mm segment prediction. This part of step 1 was inconsistent with the model prediction. In step 2 (i.e. from day 0.3 to rest of the simulations), all three simulations showed a drop in the predicted 1,3-D concentration in the top soil layer. The biggest drop was in 100 mm segment predicted value followed by 25 mm segment and 5 mm segment predicted 1,3-D concentrations, in that order. Hence, in step 2, model predictions were the inverse of the expected concentrations because predicted flux for the 100 mm segment simulation continued to be greater than the others (Figure 4a). This apparent inconsistency may be explained by soil moisture differences. Moisture in the top soil segment may act as a hindrance to volatilization. Since thin segments had lower volatilization losses, it is reasonable to hypothesize that the model would predict higher moisture content in the top layer of a thinner segment over the duration of simulation than in a thicker segment for the same duration. Figures 6a and 6b show the moisture contents of the top layer for the three simulations at 100 mm, 25 mm, and 5 mm segment thicknesses.

Figure 6a: Moisture content (v/v) in top soil segment for 100 mm, 25 mm, and 5 mm segment simulations

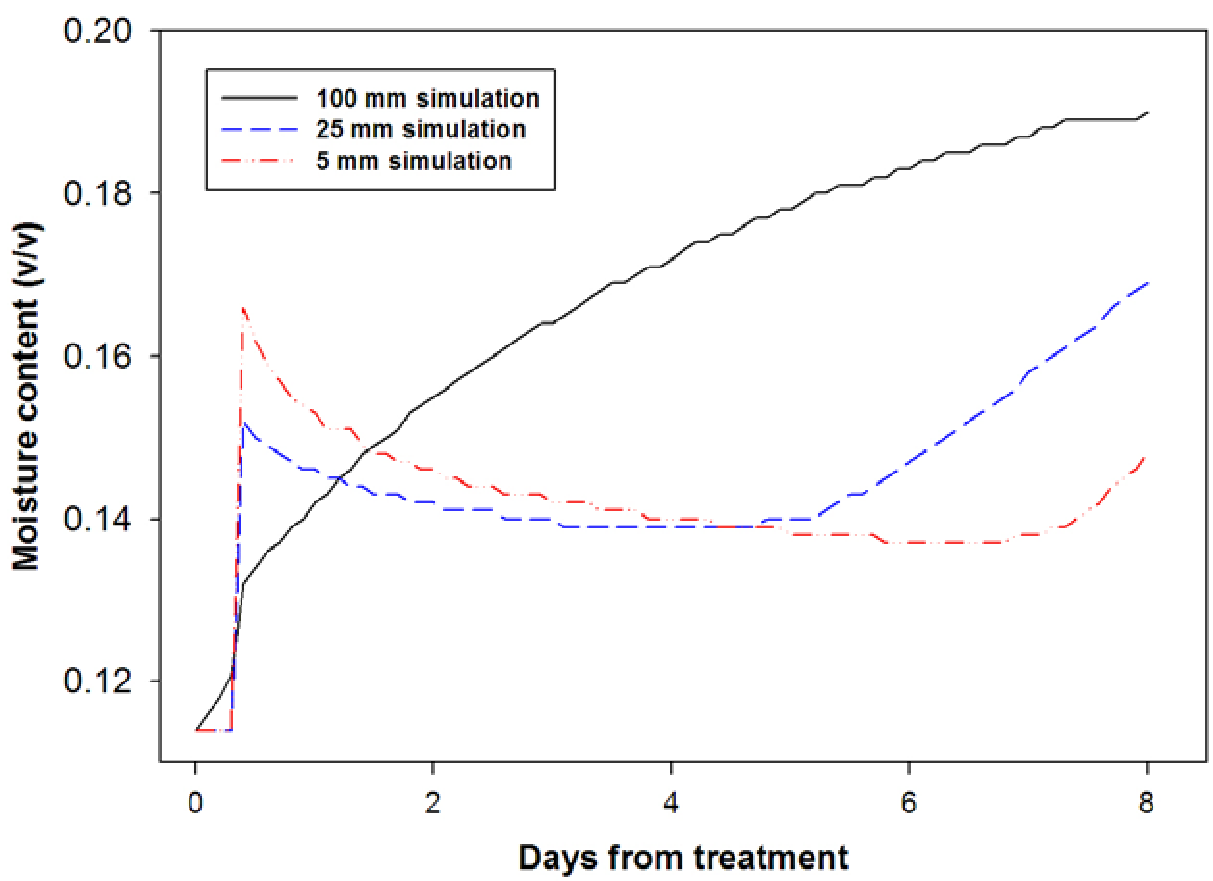
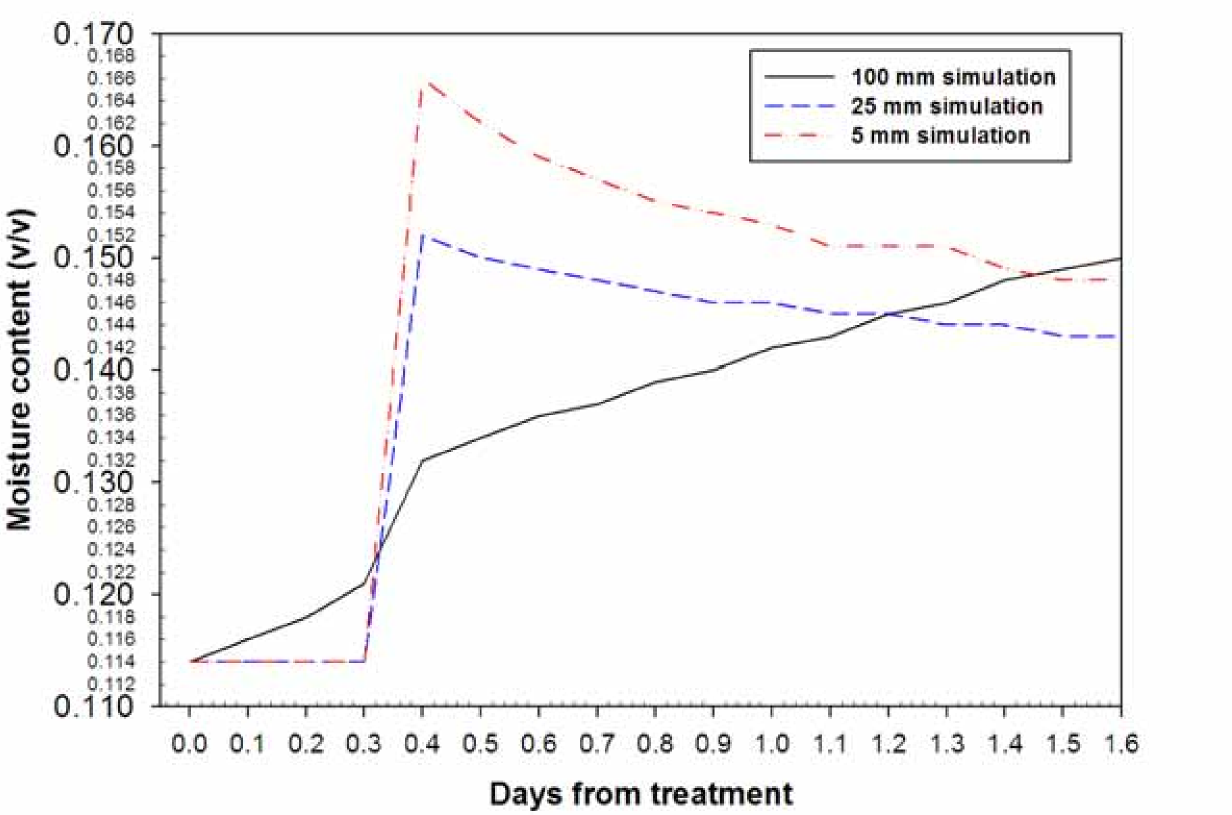


Figure 6b: Moisture content (v/v) in top soil segment for 100 mm, 25 mm, and 5 mm segment simulations zoomed to 1.6 days to show details more clearly



These plots show a mixed response relative to what was reported in Figures 5a and 5b. If the model is internally consistent, thicker segment simulations that reported larger fluxes should have lower moisture contents than the thinner segment simulations. Up to 0.3 day the moisture content in 100 mm segment was higher than the other two, which is the inverse of what would be expected based on the flux (Figure 4b). The 25 mm and 5 mm segment simulations have about the same soil moisture consistent with their similar fluxes (Figure 4b). The highest rate of change in moisture was from 0.3 to 0.4 day. After 0.4 day, the 100 mm segment moisture increased at a slower rate for the rest of the period. The two thinner segments showed a decrease. After 0.3 day to about 1.2 day, the moisture predictions were consistent with the flux pattern. Thereafter the predictions were inconsistent.

The peak simulated fluxes of 2147, 792, and 186 mg/m^2-0.1d (Figure 4b) were inversely correlated with the moisture contents at 0.4 d of 0.132, 0.152, and 0.166 (Figure 6b) for the 100 mm, 25 mm, and 5 mm segment simulations respectively. Thus it appears that the top layer water content dominated the initial peak simulated volatilization and this part of the simulation appears to be internally consistent. However, after day 2 the water content of the upper layer was highest for the 100 mm simulation (Figure 6a), which should reduce flux. Moreover, the top layer 1,3-D concentration was lowest for the 100 mm simulation, which should reduce flux, and produce conditions for the lowest flux compared to the other two simulation scenarios that had higher 1,3-D concentrations and lower water contents. However, the 100 mm simulation continued to show the highest flux after day 2 (Figure 4b). This part of the simulation seems internally inconsistent.

A sensitivity analysis of the model was performed using soil temperature data from the Imperial Valley study. Knuteson et al. (1992) reported the soil temperature at 2.5 cm, 10 cm, 30 cm, and 50 cm respectively for each day for the duration of the study. The range was 15.3 ^{0}C to 18.9 ^{0}C. The model cannot account for any changes in the degradation rate with changing soil temperature. However, the model can be set to account for the transformation rate changes with changing temperature. Using this fact, the actual degradation rate constant value was inputted at the place where transformation rate constant value should be inputted in the model. Then where the degradation rate constant value should be inputted, it was set to zero. Thus in the output file, value reported under transformation loss was actually due to degradation loss. First the model was run using the lower temperature value of 15.3 ^{0}C as the initial soil temperature of the entire profile. Another run was made by setting the initial temperature to 18.9 ^{0}C in all segments. The resulting predicted losses after 8 days were examined. With 15.3 ^{0}C, the 8-day cumulative loss was 18.85 percent of the applied 1,3-D. When the upper end, 18.9 ^{0}C was used; the 8-day cumulative loss was 18.54 percent of the applied. These were not very different from each other or from the 17.9 percent loss reported with the varying soil temperature in profile as reported in Imperial Valley study.

CONCLUSIONS

I asked two questions from this investigation. The first question was how well does the model output compare with the field measurements? The model simulated large bursts of flux at the beginning and declining flux afterwards. The measured values show much more oscillation with increasing flux peaks towards the end. Both 100 and 25 mm simulations greatly overestimated flux and the 5 mm simulation was closest with peak simulated flux within the same order of magnitude as measured. The second question was whether the model seemed internally consistent, i.e., does the simulated flux properly reflect the top layer 1,3-D concentration and water content? If internally consistent, then higher concentration should correspond with higher flux and higher water content should correspond with lower flux. In this case the model seems internally consistent for the peak flux, but not for the flux for days 2-8. Peak flux does seem to reflect the water contents that occur in the rapidly changing initial period (the top layer concentrations in this rapidly changing period are similar). However after the initial period, when the water contents and concentrations are ordered (that is the relationship between 100, 25, and 5 segments does not change), it seems inconsistent. This is because the simulation with the highest water content and lowest concentration still gives the highest flux. Therefore, it is reasonable to conclude that LEACHP version of this model is not a useful tool to predict volatilization losses from a highly volatile pesticide soil fumigant.

bcc: Gurusinghe Surname File

References

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Hutson, J. L., and R. J.Wagenet. 1992. LEACHM, Leaching Estimation and Chemistry Model version 3. Research Series No. 92-3, Dept. of Soil, Crop, and Atmospheric Sciences, Cornell University, Ithaca, NY.

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Spurlock, F., M. Clayton, and J. Troiano. 2006. Modeling Herbicide Movement to Ground Water in Irrigated Sandy Soils of the San Joaquin Valley, California. Water, Air and Soil Pollution 176: 93-111.

Troiano, J., C. Garretson, C. Krauter, J. Brownell, and J. Hutson. 1993. Influence of Amount and Method of Irrigation Water Application on Leaching of Atrazine. J. of Environ. Qual. 22:290-298.

Appendix 1

pg10c < Filename: 8 characters with no extension. Used in batch runs (started as LEACHP<filename>).

LEACHP PESTICIDE DATA FILE.
A value must be present for each item, although it may not be used in this
simulation. The file is read free format with blank delimiters. Preserve
division and heading records. The number of depth segments may be changed.
****

1 <Date format (1: month/day/year; 2: day/month/year). Dates must be 6 digits, 2 each for day, mo, yr.
021891 <Starting date. No date in the input data should precede this date.
000030 <Ending date or day number. The starting date is day 1. (A value <010101 is treated as a day number).
0.05 <Largest time interval within a day (0.1 day or less).
1 <Number of repetitions of rainfall, crop and chemical application data.
1000 <Profile depth (mm), preferably a multiple of the segment thickness.
100 <Segment thickness (mm). (The number of segments should be between about 8 and 30.
2 <Lower boundary condition: 1:fixed depth water table; 2:free drainage, 3:zero flux 4:lysimeter.
0000 <If the lower boundary is 1 or 4: initial depth to water table (mm).

The steady-state flow option uses constant water fluxes during the application
periods specified in the rainfall data table, and a uniform water content
specified here. Steady-state flow implies a lab column, and crop and evaporation data are ignored.

----

1 < Water flow: 1: Richards; 2: Addiscott tipping bucket; 3: steady-state (no crops assumed).
0.4 < Steady-state flow water content (volume fraction); 999: saturated column.
****

****

2 <Number of output files: 1: OUT only; 2: OUT + SUM; 3: OUT + SUM + BTC

--- For the *.OUT file :
2 <Units for depth data: 1: ug/kg, 2: mg/m2 per segment depth, 3: mg/kg, 4: g/m2, 5: kg/ha.
1 <Node print frequency (print data for every node (1), alternate nodes (2).
2 <Print option: 1 or 2. Use to specify one of the following options.
1 <Option 1: Print at fixed time intervals (days between prints).
81 <Option 2: No. of prints (the times for which are specified below)
2 <Tables printed: 1: mass balance; 2: + depth data; 3: + crop data
0 <Reset cumulative values in .OUT file after each print? 0: No, 1: Yes

----

--- For the * .SUM file :
.1 <Summary print interval (days) (for calendar months use 999)
100 <Surface to [depth 1?] mm (Three depth segments for the
200 <Depth 1 to [depth 2?] mm summary file. Zero defaults to nodes
300 <Depth 2 to [depth 3?] mm closest to thirds of the profile)
3 <4th segment: Root zone (1); profile (2); Depth 3 to lower boundary (3); Surface to shallowest of lower boundary or water table (4)

--- For the *.BTC (breakthrough) file :

```
 1.0    <Incremental depth of drainage water per output (mm)
------------------------------------------------------------------------
-- List here the times at which the *.OUT file is desired for print option 2.
-- The number of records must match the 'No. of prints' under option 2 above.
       Date or    Time of day         (At least one must be specified
       Day no.  (to nearest tenth)      even if print option is not 2)
       --------  ----------------

            021891        .0       (These dates can be past the last day)
            021891        .1       (These dates can be past the last day)
            021891        .2       (These dates can be past the last day)
            021891        .3       (These dates can be past the last day)
            021891        .4       (These dates can be past the last day)
            021891        .5       (These dates can be past the last day)
            021891        .6       (These dates can be past the last day)
            021891        .7       (These dates can be past the last day)
            021891        .8       (These dates can be past the last day)
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            021991        .1       (These dates can be past the last day)
            021991        .2       (These dates can be past the last day)
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            022091        .1       (These dates can be past the last day)
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            022191        .9       (These dates can be past the last day)
            022191        1       (These dates can be past the last day)
            022291        .1       (These dates can be past the last day)
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022291 .2 (These dates can be past the last day)
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022291 .9 (These dates can be past the last day)
022291 1 (These dates can be past the last day)
022391 .1 (These dates can be past the last day)
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022591 .1 (These dates can be past the last day)
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022591 1 (These dates can be past the last day)

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****

SOIL PHYSICAL PROPERTIES Retention models - 0: listed Campbell parameters;
Campbell + pedotransfer functions (see Table 3.2): 1: SA Cl+Si; 2: SA Cl;
3: UK topsoils; 4: UK subsoils; 5: USA Rawls and Brakensiek;
6: listed van Genuchten parameters (use e.g. RETC to estimate these).

```
 Soil |                 |Retention|   Starting   |   Roots   | Starting
layer | Clay  Silt  Organic |  model  |theta or pot'l|  (for no  | temp (C)
 no.  |           carbon  |         |(one is used) |  growth)  | (not read in
      |  %     %     %    |         |          kPa | (relative)|  LEACHC)
```

---	----	----	----	------	-----	-----	------	-----------
1	28.7	39.5	0.55	5	0.114	-10	0.20	15.7
2	27.1	42.6	0.40	5	0.162	-10	0.20	16.5
3	25.5	45.7	0.24	5	0.209	-10	0.15	16.5
4	19.8	50.6	0.15	5	0.213	-10	0.13	17.2
5	18.1	48.8	0.14	5	0.213	-10	0.1	17.2
6	16.3	47.0	0.12	5	0.213	-10	0.08	17.3
7	16.8	47.4	0.11	5	0.213	-10	0.05	17.3
8	16.1	45.0	0.10	5	0.213	-10	0.04	17.3
9	15.3	42.5	0.08	5	0.213	-10	0.02	17.3
10	15.3	42.5	0.08	5	0.213	-32	0.02	17.3

----

1 < Use listed water contents (1) or potentials (2) as starting values.

Particle density: Clay Silt and sand Organic matter (kg/dm3) (to calculate porosity)

2.65 2.65 1.10

****

For a uniform profile: Non-zero values here will override data in the next
table of depth-specific data.

0.0 0.00 :if >0, Soil bulk density and particle density (kg/dm3).

-0.0 :if <0, Campbell 'Air-entry value' (kPa), or van Genuchten alpha (kPa^-1).

0.0 :if >0, Campbell exponent b, or van Genuchten n.

2019.0 -0.5 :if K>0, Conductivity (mm/day) and corresponding matric potential (kPa) (for potential-based version of eq. Retfun 5).

1 :if >0, Campbell pore interaction parameter or van Genuchten residual saturation.

48.8075123 :if >0, Dispersivity (mm).

-10 :if >0, For Addiscott flow: Matric potential (kPa) at field capacity

-200 :if >0, : Division between mobile and immobile water (kPa)

****

Soil segment no.	Retention function parameters CHC: AEV / vG: alpha	CHC: BCAM / vG: n	Bulk density kg/dm3	K matching factor mm/d	potl kPa	CHC: P vG: ResSat	Dispersivity mm	For Addiscott flow option: Field capacity kPa	Mobile/immobile threshold kPa
-----	------	-----	------	----	-----	-----	-----	------	---------
1	-0.01644	5.1910	1.33	1	-15	3	30	-5.0	-200.
2	-0.01644	5.1910	1.39	1	-15	3	30	-5.0	-200.
3	-0.01644	5.1910	1.44	1	-15	3	30	-5.0	-200.
4	-0.01644	5.1910	1.37	1	-15	3	30	-5.0	-200.
5	-0.01644	5.1910	1.33	1	-15	3	30	-5.0	-200.
6	-0.01644	5.1910	1.29	1	-15	3	30	-5.0	-200.
7	-0.01644	5.1910	1.29	1	-15	3	30	-5.0	-200.
8	-0.01644	5.1910	1.29	1	-15	3	30	-5.0	-200.
9	-0.01644	5.1910	1.29	1	-15	3	30	-5.0	-200.
10	-0.01644	5.1910	1.29	1	-15	3	30	-5.0	-200.

****

****

Runoff according to the SCS curve number approach. Curve number listed here will be

```
adjusted by slope. During periods of crop growth, CN2 replaced by value for crop.
(Procedure according to J.R. Williams (1991). Runoff and Water Erosion.
Chap 18, Modeling Plant and Soil Systems, Agronomy 31.)
----------------
 75   <Curve number (CN2).  In LEACHM, water content use to adjust CN2 based on top 20 cm.
 0    <Slope, %. Used to adjust CN2 according to equation of Williams (1991).
** (Set slope to 0 to bypass the runoff routine.  Runoff owing to profile saturation will still be accumulated)
****************************************************************************
****************************************************************************
                    CROP DATA
----------------------------------------------------------------------
  Data for at least one crop must be specified, even if no crop desired.
  For fallow soil, set flag below to 0, or germination past the simulation end date.
----------------------------------------------------------------------
0      <Plants present: 1 yes, 0 no.  This flag overrides all other crop data.
1      <Number of crops (>0, even if bypassed).  Dates can be past last day of simulation.
-1500  <Wilting point (soil) kPa.
-3000  <Minimum root water potential(kpa).
1.1    <Maximum ratio of actual to potential transpiration (dry surface).
1.05   <Root resistance (weights water uptake by depth). (>1, No weighting: 1.0).
------------------------------------------------------------------------------------------------------------------------------
Growth  Perennial  N_uptake           Date or day of         Rel.  Max crop   Crop    Mulch     ETp  |  Crop    Min
Harvested
1: No   1: Yes   1:to maturity                Maturity        root   cover   cover at  effect  scaling| uptake    N    fraction
2: Yes  2: No    2:to harvest  Germ. Emerg.   Root  Cover  Harv. depth fraction  harvest    %      factor|  N   P   fixed
------  -------  ------------  -------------------------------- -----  ------  ----       ---     ----    -----kg/ha---- ----------
  2       1          1     031595  031695 061595 061595 101595  2.00   0.8       0.8     000     1.00    102  20   0     .88
**********************************************************************************************************
*************************************
****************************************************************************
                 INITIAL PROFILE CHEMICAL DATA
----------------------------------------------------------------------
   1    < Number of chemical species.  At least one must be specified.
----------------------------------------------------------------------
 Soil    Chem1    Chem2    Chem3     Chem4 .. (Add columns to match number of chemicals)
layer        ----mg/kg dry soil----
----------------------------------------------------------------------
  1       0        0        0       0
  2       0        0        0       0
  3       0        0        0       0
  4       0        0        0       0
  5       94.45    0        0       0
  6       0        0        0       0
  7       0        0        0       0
  8       0        0        0       0
  9       0        0        0       0
 10        0        0        0       0
----------------------------------------------------------------------
Concentration (mg/l) below profile, used with lower boundaries 1 or 5. (Extend record to match number of chemicals)
                          0.0       0.0       0.0       0.0      0.0
```

```
0    < Depth (mm) of water in mixing cell (boundaries 1 and 5 only). Enter 0 for no mixing cell.
***********************************************************************
***********************************************************************
                        CHEMICAL PROPERTIES
                        -------------------
Chem              Solubility  Vapour Density    Link       Plant
 No.      Name       mg/dm3       mg/dm3     (No:0 Yes:1)   Uptake
-------    ----       ------       --------     -------    1(yes),0(no)
  1    ' 1, 3 dich  '     2320          4540        100          0
----------------------------------------------------------------------
      Linear(1)     |      Linear isotherm     | Freundlich isotherm
Chem     or         |  Koc    2-site model    |  Kfoc  Exponent
 No.  Freundlich(2)  |  l/kg    f      alpha    | (unit dependent!)
----   -----          -----   ---    ------      ------     ---
  1       1           27.66   1.0      .693        100     1.0
-------------------------------------------------------------------------
Diffusion coefficients:
--------------------
 120       <Molecular diffusion coefficient in water (mm2/day)
 .4300E+06 <Molecular diffusion coefficient in air (mm2/day)
 .1400E+06 <Air diff. coeff. enhancement to account for atmospheric pressure fluctuations.
***********************************************************************
*  The values of L1,L2--->Ln ('Link' in the Chemical Properties above)
*   determine which species form a transformation chain. Setting 'Link'
*   to 0 breaks the pathway, setting 'Link' to 1 restores it.
*
*                  Transformation pathways------------------->
*    |    RATE 1         RATE 2         RATE 3         RATE 4
*   Chem1---/L1/--->Chem2---/L2/--->Chem3---/L3/---Chem4---/L4/--->...
*    |            |             |            |
*    | RATE 5       | RATE 6       | RATE 7       | RATE 8    Degradation
*    |            |             |            |            pathways
*    v            v             v            v             |
*  PRODUCT       PRODUCT       PRODUCT       PRODUCT           |
*                                                        v
****************************************************************************
                 TRANSFORMATION AND DEGRADATION RATE CONSTANTS
--------------------------------------------------------------------------
 1 <Apply rate constants to (0) solution phase only, (1) solution AND sorbed phases (excluding precipitate)
-- Temperature and water content affects (transformation rate constants only):
    0   <Rate constants: Temperature and water adjustments: no(0), transformation only (1), trans and degradation (2)
    4.1   <Q10: factor by which rate constant changes per 10 C increase
   20   <Base temperature: at which rate constants below apply
   35   <Optimum temperature: Q10 relationship applies from 0 C to here
   50   <Maximum temperature: Rate constants decrease from optimum to here
  .1   <High end of optimum water content range: air-filled porosity
 -300   <Lower end of optimum water content: matric potential kPa
-1500   <Minimum matric potential for transformations kPa
  1.0   <Relative transformation rate at saturation
*************************************************************************
```

TRANSFORMATION RATE CONSTANTS (may be adjusted as specified above)

Layer no	Chemical 1	Chemical 2	Chemical 3	Chemical 4 ......
---------	<---------------------	day^(-1)	--------------------->	
1	0.000	0	0	0
2	0.000	0	0	0
3	0.000	0	0	0
4	0.000	0	0	0
5	0.000	0	0	0
6	0.000	0	0	0
7	0.000	0	0	0
8	0.000	0	0	0
9	0.000	0	0	0
10	0.000	0	0	0

****

DEGRADATION RATE CONSTANTS (not influenced by water or temperature)

Layer no	Chemical 1	Chemical 2	Chemical 3	Chemical 4 ....
---------	<---------------------	day^(-1)	--------------------->	
1	0.11	0	0	0
2	0.11	0	0	0
3	0.11	0	0	0
4	0.11	0	0	0
5	0.11	0	0	0
6	0.11	0	0	0
7	0.11	0	0	0
8	0.11	0	0	0
9	0.11	0	0	0
10	0.11	0	0	0

****
****

CHEMICAL APPLICATIONS

1 < Number of broadcast applications. (At least 1. Can be past last date.

Date (or day no.)	Incorporation (segments, 0 is surface)	Chem1	Chem2	Chem3	Chem4 ....
		mg/sq.m (1mg/sq.m = .01kg/ha)			
-----		--------	-----	-----	-----
021991	5	0.00	0.00	0.00	0.00

****
****

CULTIVATIONS

1 < Number of cultivations. At least one must be specified. Can be past last day.

Date or day no.	Depth of cultivation mm
-------	-----

```
 9999        200
*************************************************************************
*************************************************************************
     RAIN AND RAIN WATER COMPOSITION  (Include irrigation here, or specify
     -------------------------------    in a separate file.)
  1 < Number of water applications.  Some or all can be past last day. (See manual on setting automated irrigation thresholds)
  0 < For a separate irrigation file, set to 1 and edit and rename PESTTEST.SCH.
-------------------------------------------------------------------------
     Start      Amount  Surface flux      Dissolved in water (can be 0)
Date/day  Time            density     Chem1     Chem2    Chem3    Chem4.....
-------  --day-  --mm--  ---mm/d----  ---------------  mg/l  -------------
021891     .3     1.0     260.0    0.00   0.00    0.00   0.00
*************************************************************************
*************************************************************************
  REFERENCE ET (WEEKLY TOTALS, mm), DEPTH TO WATER TABLE (mm)  (Note: Lower boundary conditions 1 to 4 read, but do not use the water table depth data)
  MEAN WEEKLY TEMPERATURES AND MEAN WEEKLY AMPLITUDE (degrees C)
-------------------------------------------------------------------------
     Week no. Ref.ET Water table   Mean temp  Amplitude
     --------------------------------------------------
          1      25.146     1500      15.3    10.0
          2      25.146     1500      15.3    10.0
          3      25.146     1500      15.3    10.0
          5      25.146     1500      15.3    12
          6      25.146     1500      15.3    12
          7      25.146     1500      15.3    12
          8      25.146     1500      15.3    12
          9      25.146     1500      15.3    12
     10      25.146     1500      15.3    12
     11      25.146     1500      15.3    12
     12      25.146     1500      15.3    12
     13      25.146     1500      15.3    12
     14      25.146     1500      15.3    12
     15      25.146     1500      15.3    12
     16      25.146     1500      15.3    12
     17      25.146     1500      15.3    12
     18      25.146     1500      15.3    12
     19      25.146     1500      15.3    12
     20      25.146     1500      15.3    12
     21      25.146     1500      15.3    12
     22      100.00     1500      21.53   12
     23      100.00     1500      21.84   12
     24      100.00     1500      23.25   12
     25      100.00     1500      24.33   12
     26      100.00     1500      24.70   12
     27      100.00     1500       5.57   12
     28      100.00     1500      26.76   12
     29      100.00     1500      26.03   12
     30      100.00     1500      26.30   12
```

31	100.00	1500	26.43	12
32	100.00	1500	26.67	12
33	100.00	1500	25.83	9.00
34	100.00	1500	24.90	9.14
35	100.00	1500	25.60	9.09
36	100.00	1500	24.87	9.04
37	100.00	1500	22.93	8.95
38	100.00	1500	22.66	8.77
39	100.00	1500	21.65	8.31
40	100.00	1500	20.77	8.81
41	25.146	1500	19.28	8.93
42	100.00	1500	17.77	8.91
43	100.00	1500	16.58	8.10
44	100.00	1500	14.38	7.51
45	100.00	1500	13.43	7.52
46	100.00	1500	11.52	6.60
47	100.00	1500	10.60	6.27
48	100.00	1500	9.34	6.18
49	100.00	1500	9.20	6.03
50	100.00	1500	7.87	5.22
51	100.00	1500	6.40	4.68
52	100.00	1500	6.27	5.06
53	100.00	1500	7.40	4.51