EVALUATION OF HYDRUS FOR SIMULATING FUMIGANT VOLATILIZATION AND TRANSPORT

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Field fumigant studies are expensive to conduct, and associated flux estimation methods are subject to considerable uncertainty. Alternately, mechanistic simulation models may be used to estimate flux, but few (if any) models have been shown to accurately describe the full range of fumigant fate and transport processes in soil. This paper summarizes the California Department of Pesticide Regulation's initial test of HYDRUS 2D/3D as a tool to estimate fumigant transport and volatilization in the field.

In 2011, a field study was conducted in Lost Hills, CA. In that study, 3 fields of Milham sandy loam were fumigated with approximately 300 lbs/acre of Pic-Chlor 60 under a totally impermeable film (TIF) tarp (Ajwa et al., 2013). Tarp-cut times were 16 days (field 1), 10 days (field 2) and 5 days (field 3). A primary objective of that study was to determine appropriate tarp-cutting times for the TIF tarp. Chloropicrin (CP) and 1,3-dichloropropene (13D) field-estimated fluxes were determined using the back-calculation method with the Industrial Source Complex – Short Term version 3 dispersion model (ISC).

A second objective in the Lost Hills study was to generate data for evaluating the HYDRUS 2D/3D model for simulating fumigant transport and volatilization. Three variables that have a strong impact on modeled flux are difficult to accurately measure or estimate: (1) field effective TIF tarp mass transfer coefficient (MTC), (2) fumigant soil sorption coefficient (K_{OC}), and (3) fumigant soil half-life. Therefore, field 1 ISC flux estimates for CP and 13D, and measured soil-gas and soil properties data were used to calibrate HYDRUS. This was achieved by optimizing the three variables to obtain best agreement between model-predicted and field-based flux and measured under-tarp soil gas concentrations (Spurlock et al., 2013). All remaining model input data were either measured directly or independently estimated. Model "validation" simulations then consisted of HYDRUS simulation of fields 2 and 3 with no further adjustment of any input variables, i.e. all model inputs were taken from the previous calibration procedure, estimated or directly measured in fields 2 and 3.

Calibration Results. Best-fit fumigant half-lives and K_{OC}s (Table 1) were well within the range of literature estimates for these parameters. However, the fitted effective field TIF MTC were much higher than laboratory measurements made on fresh unused tarp as has been previously reported in other studies. They were, however, comparable to laboratory MTC measurements made on post-tarpcut TIF samples from the Lost Hills study (Spurlock et al., 2013). The maximum HYDRUS discrete time-weighted average flux densities and cumulative fluxes were within the estimated range of uncertainty of the ISC estimates, and demonstrated similar diurnal fluctuations (Figure 1). Soil-gas concentrations (Figure 2), and end-of-study soil water content and temperature with depth (not shown) agreed very well with field measured values, indicating the individual processes of fumigant air-water-soil partitioning, soil-water dynamics and heat transport were reasonably well-described by the calibrated HYDRUS 2D/3D model.

Validation Results The magnitudes of the discrete HYDRUS flux estimates for fields 2 and 3 also agreed well with the ISC field-based estimates (Figures 3 and 4), as did the cumulative flux profiles. However, as in the calibration field 1 case, while the magnitudes of the simulated CP and 13D *maximum* discrete fluxes agreed well with the ISC estimates, they were generally delayed by 1-2 days (Figures 1, 3). There are several possible reasons for these systematic differences (Spurlock et al., 2013). Finally, HYDRUS estimates for the maximum post-tarpcut discrete fluxes agreed well with the ISC estimates (Figure 4).

Conclusion In this study, the calibrated HYDRUS model yielded flux estimates comparable in magnitude to the standard ISC "back-calculation" procedure. The soil-gas, soil temperature and end-of-study water content data indicate that the calibrated model described individual fumigant, water and heat transport processes accurately; i.e. the model approximated reality. However, the timing of the peak discrete fluxes was delayed relative to ISC estimates. Among the 3 calibrated variables, the field effective TIF MTC is the most difficult to estimate due to a lack of empirical TIF MTC data.

References

Ajwa, H., M. Stanghellini, S. Gao, D.A. Sullivan, A. Khan and R. Qin. 2013. Fumigant emission reduction using totally impermeable film. Calif. Agric., *in press*.

Spurlock, F., B. Johnson, A. Tuli, S. Gao, J. Tao, F. Sartori, R. Qin, D. Sullivan, M. Stanghellini and H. Ajwa. 2013. Simulation of Fumigant Transport and Volatilization from Tarped Broadcast Applications. Vadose Zone J., *in press.* doi:10.2136/vzj2013.03.0056

Table 1. Field 1 HYDRUS chloropicrin (CP) and 1,3-dichloropropene (13D) calibration results: optimized variables (95% Confidence Interval)

variable	CP	13D
fumigant half-life (d)	4.3 (3.9, 4.8)	7.2 (6.7, 7.6)
Soil sorption coeffic. K_{OC}	66 †	30 †
field effective TIF MTC (cm h^{-1})	0.12 (0.11, 0.14)	0.22 (0.20, 0.23)

† Confidence intervals not determined

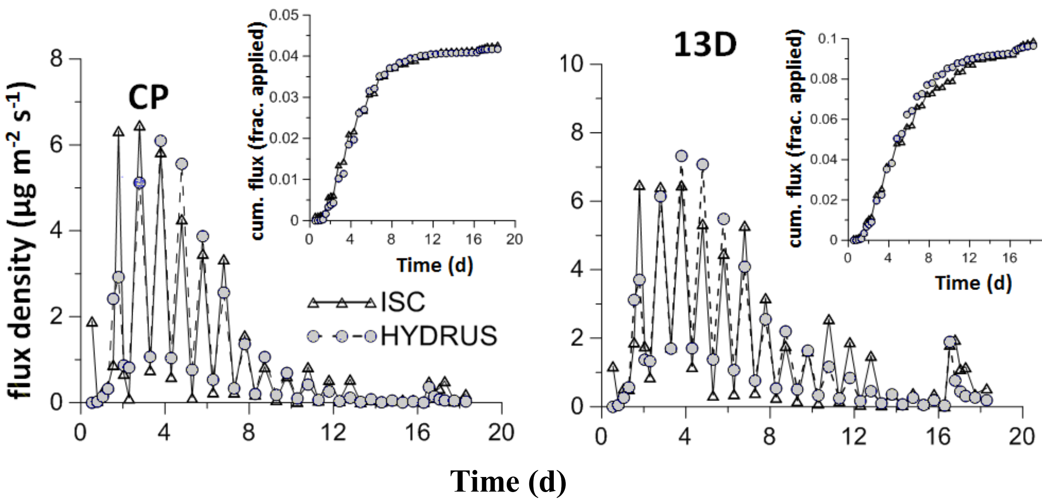

Figure 1. Calibration field 1 HYDRUS-predicted and ISC field-estimated CP and 13D discrete time average flux densities and cumulative fluxes.

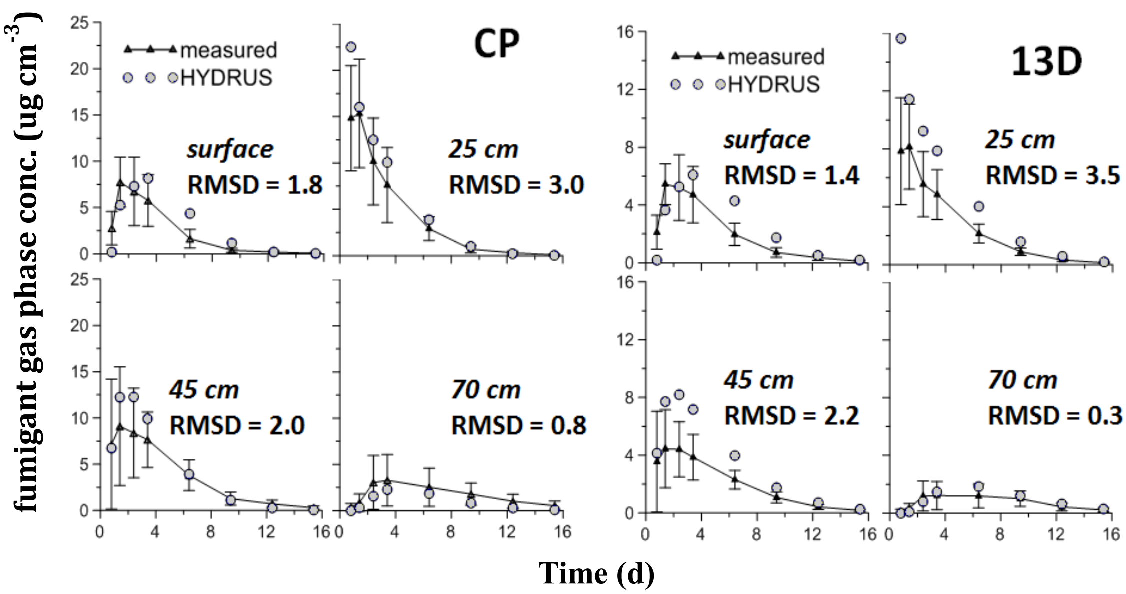

Figure 2. HYDRUS-predicted and measured CP and 13D soil-gas concentrations at different depths in field 1 profile. Note: only surface (sub-tarp, depth = 0) samples were used to calibrate model; RMSD = root mean square deviation. Each time, N=12 for surface samples, N=24 all other depths.

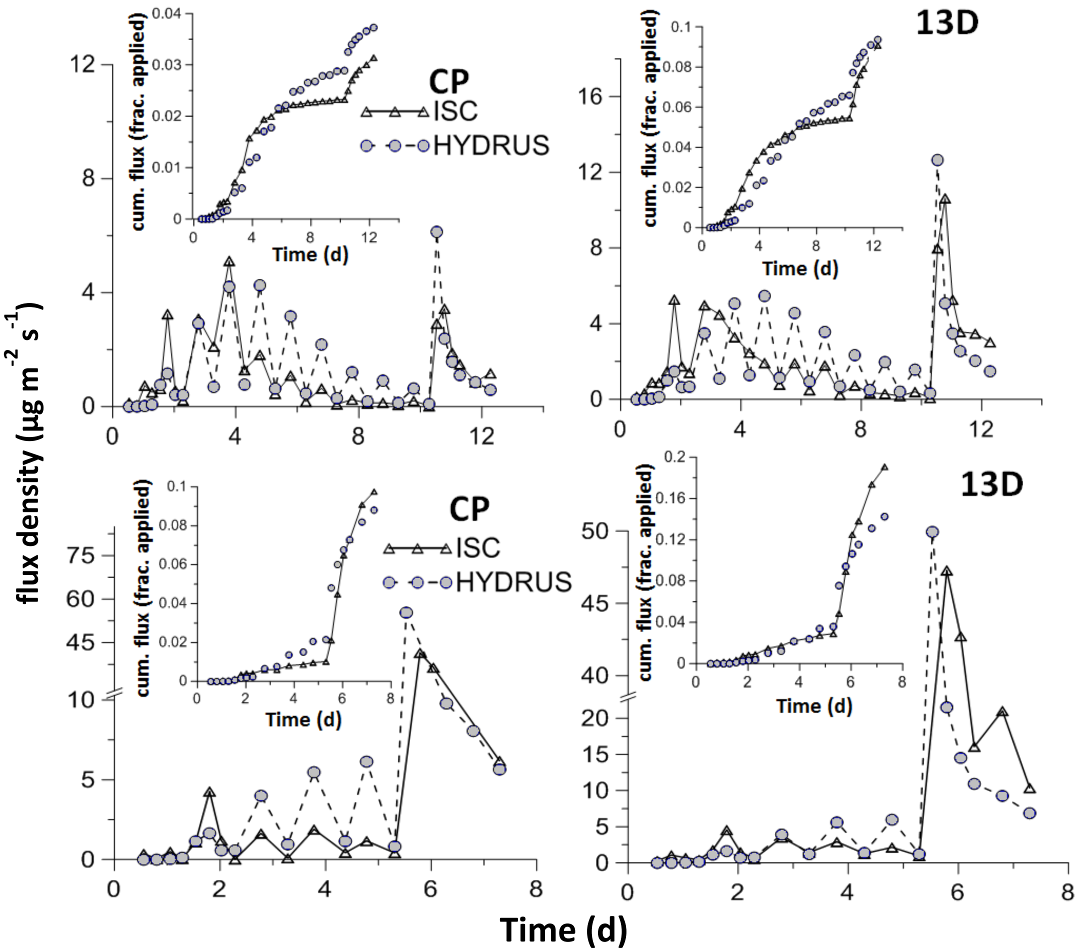

Figure 3. Field 2 (top) and Field 3 (bottom) HYDRUS-predicted and ISC field-estimated CP and 13D discrete time average flux densities and cumulative fluxes. Tarpcut times: field 2, 10d; field 3, 5 days. Note broken Y-axes on field 3 plots.

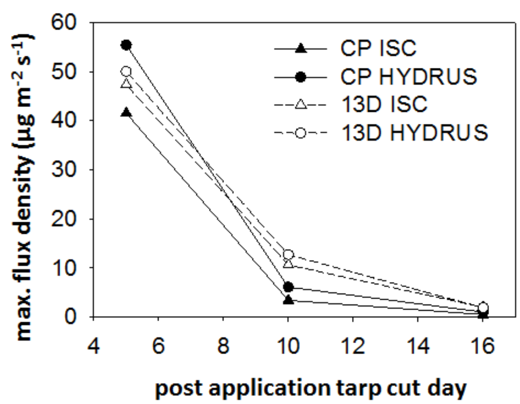

Figure 4. Comparison of HYDRUS-predicted and ISC-estimated maximum post-tarpcut discrete flux densities vs tarpcut day.