PREDICTING THE FATE OF IMIDACLOPRID IN A COASTAL PLAIN SETTING USING VS2DT

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Abstract. Imidacloprid has been shown to control pine tip moths (*Rhyacionia* spp.) in loblolly pine seedlings (*Pinus taeda* L.). We describe an imidacloprid dissipation study on a small watershed near Downs, Georgia. Field data are utilized to calibrate the computer model VS2DT (Variably Saturated 2-Dimensional Transport) that uses a finite-difference approximation of the advection-dispersion equation to simulate contaminant transport through variably saturated porous media. The site is simulated in a vertical cross section (X-Z plane) of a treated watershed from the soil surface to the water table (approximately 60 ft) spanning 260 ft horizontally. The cross section is centered on an ephemeral stream which drains the watershed, but for symmetry reasons, only half (130 ft horizontal distance) of the cross section is modeled. Modeling results show that imidacloprid moves more rapidly through sandy soils than sandy clay loam soil material. No imidacloprid concentrations above the detection limit of 0.6 ppb are predicted for the lysimeters in the unsaturated zone or in groundwater.

INTRODUCTION

Infestation by pine tip moths (*Rhyacionia* spp.) is one of the limiting factors in early growth and development of pine stands in the Southeastern United States. Imidacloprid (1-[(6-chloro-3-pyridinyl)-methyl]-4,5-dihydro-*N*-nitro-1H-imidazol-2-amine) is a systemic insecticide which has shown efficacy in controlling sucking insects, some beetles, weevils and leafminers on various crops. Imidacloprid applied in a Florida field study controlled tip moths on loblolly pine seedlings (*Pinus taeda* L.) for 1-3 years (Foltz, 1994).

An imidacloprid environmental fate study was initiated in January, 1996 on a coastal plain site near Downs, Georgia. Imidacloprid residues in runoff-water, soil solution and groundwater are monitored after significant rainfall events. This residue data is used to assess the VS2DT hydrologic model.

The fate and transport of pesticides depend on the flow path within the soil. There are three major flow paths: overland flow, subsurface lateral flow, and vertical percolation through the unsaturated zone to the water table. Overland flow rarely occurs within forested watersheds. Solute transport through the subsurface is controlled by various mechanisms including advective transport (Solutes are moving with the flowing water.), hydrodynamic dispersion (Variability of fluid velocity causes a spreading of solutes toward the average direction of water flow.), and solute sorption. Solute transport is also dependent on the soil structure because interconnected macropores induce preferential flow paths which accelerate the movement of solutes.

Computer models have been developed to simulate the fate of pesticides because environmental fate studies are expensive and time consuming. Hydrologic computer models for water and solute movement within variably saturated porous media are useful tools for gaining insight into processes that occur within the unsaturated zone. A hydrologic environmental model, VS2DT (Variably Saturated 2-Dimensional Transport) has been developed by the U.S. Geological Survey. This model uses a finite-difference approximation to the advection-dispersion equation to simulate water movement through variably saturated porous media. VS2DT can simulate problems in 1-dimensional columns, 2-dimensional vertical cross sections (X-Z plane), or 3-dimensional, axially symmetric cylinders (Healy, 1990 and Healy *et al*, 1993). Boundary conditions used for flow include fixed pressure heads, infiltration with ponding, evaporation from the soil surface, plant transpiration, or seepage faces.

OBJECTIVES

The objectives of this study are to:

1) Evaluate VS2DT's simulation of imidacloprid movement in a coastal plain watershed by comparing field data to the predicted values from VS2DT.
2) Determine limitations using VS2DT to predict pesticide movement.

MATERIALS AND METHODS

Study site

The imidacloprid study area is located in the Georgia Coastal Plain near the town of Downs in Washington County, approximately 90 miles south of Athens, Georgia. Historically, the area was a natural forest and pesticides have not been applied to the study area for at least 40 years. The imidacloprid site is surrounded by mature mixed hardwood and loblolly pine forests. A stream borders the site on the southwestern side. The stream flows from the northwest to the southeast and has a width of approximately 15 ft and depth of 2 to 4 ft.

The soil is predominately Orangeburg series with small areas of Ochlocknee series in the draws. Coastal Plain soils of the Orangeburg series are generally well drained, permeable soils of sedimentary origin. The upland flats have three distinct soil layers based on split spoon samples taken during well installation on site. The upper layer is approximately 3 to 4 ft thick and has a sandy to loamy sand texture. The middle layer is clay-enriched and consists of red, dense sandy clay to sandy clay loam that is approximately 15 to 17 ft thick. Visual observations of a nearby road cut showed rainfall-related saturation on top of the sandy clay loam layer. The final layer extends from the bottom of the red clay-enriched layer to the water table and has the same characteristics as the first horizon with a distinct bedding of sand. The watershed was created by massive erosion that exposed the red clay-enriched layer at certain areas within the site. Three-dimensional pictures of the red layer within the watershed were constructed using observations taken during the installation of lysimeters. The clay layers slope toward the center of the watershed and have erosional features hidden by overlying sand. These irregularities could aid in concentrating the insecticide within the site.

Within the imidacloprid study area, a small watershed was chosen to monitor the fate of imidacloprid. Also, an ephemeral stream forms and drains the bottom of the watershed during large rainfall events. The watershed was treated with imidacloprid and modeled using VS2DT.

Site preparation

Trees on site were harvested during August, 1994. Site and regeneration activities included spot raking (June 2, 1995), chopping using a drum roller (June 30, 1995), burning (July 14, 1995) and harrowing (September 12, 1995). On November 7, 1995, loblolly pine seedlings were planted using a mechanical planter along the contour of the watershed in a 6 ft by 12 ft spacing (600 trees/acre). Imidacloprid was applied on February 26, 1996, followed by hexazinone/sulfometuron methyl herbicide applications on April 1, 1996 and imazapyr application on September 24, 1996.

Instrumentation of the treated watershed

The 5.4 acre treated watershed is instrumented with (Figure 1):

1) a weather station equipped with a pyranometer, an anemometer, a weather vane, a relative humidity gauge, an internal and external temperature gauge, a barometer, a tipping-bucket rain gauge, a standard rain gauge, and an evaporation pan
2) 42 porous cup lysimeters for sampling soil water in unsaturated conditions
3) five 2 in diameter PVC wells for monitoring and sampling groundwater
4) a 1.5 ft H-Flume equipped with an FW-1 stage-height recorder for determining runoff volume and duration.

Insecticide application

On February 26, 1996, approximately one gram of active ingredient imidacloprid was placed 4 to 6 in in the ground to the right of each tree (4 in away from the seedling) within the treated watershed.

FIELD DATA

Field data collection began before the imidacloprid was applied to the treatment site and will continue through the next year. Monitoring rainfall, runoff volume and surface flow duration through an H-Flume for the period of March through September, 1996, allowed calculation of input-runoff ratios. Results show that only an average of 3 percent of the total volume of rainfall on the watershed flows through the H-Flumes. Based on this observation, the major pathway which imidacloprid will travel is through the vadose zone to the water table. This assumes that the pesticide does not biodegrade, adsorb strongly to organic matter and clay, or get totally absorbed systemically by vegetation.

Lysimeters and monitoring wells are used to measure the concentration of imidacloprid as it travels through the unsaturated zone to the water table. Lysimeters are located in a 6 by 6 grid and are sampled after every significant rainfall event (> 0.5 in). The lysimeters account for horizontal movement and any preferential flow paths above the clay-enriched layer. Five monitoring wells are sampled once a month to measure for groundwater contamination. Imidacloprid was not detected (detection limit = 0.6 ppb) in groundwater.

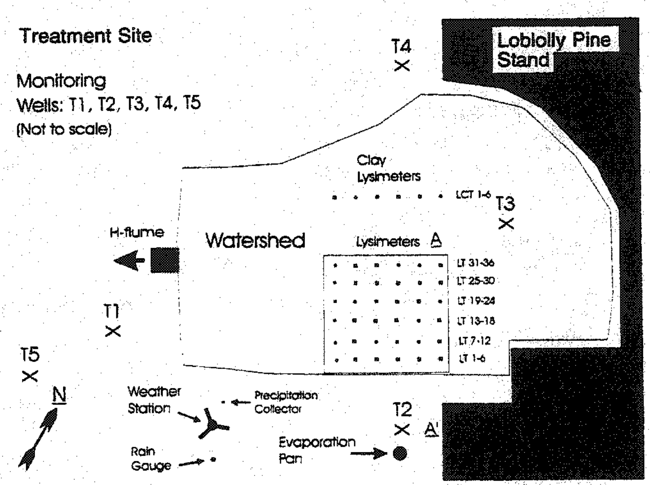

Figure 1. X-Y view of the treated watershed and the position of the monitoring devices.

CONCENTRATION CALCULATIONS

Imidacloprid concentrations for the application scoop (71 cm^3) and 15 cm of soil (304 cm^3) are calculated to calibrate the model output. Total concentration is the aqueous phase concentration plus the concentration adsorbed to the soil. The imidacloprid concentration (active ingredient) in the formulation material is 25,000 ppm. The theoretical concentration in the top 15 cm soil core is 1,890 ppm (assuming the whole application area is sampled). The initial total imidacloprid concentration in the 0-15 cm range from the model should be consistent with the value calculated for the total concentration in a 15 cm core.

MODEL DESCRIPTION

VS2DT is used to simulate the fate of imidacloprid in the treated watershed. This model is governed by the advection-dispersion and conservation of mass equations. The values for the model are approximated by a 2-dimensional, block-centered, finite-difference scheme.

VS2DT utilizes rainfall events to introduce water into the problem. Rainfall events are considered recharge events, and the times between are considered evaporation events. Data from a tipping-bucket rain gauge is used to calculate the duration and intensity of the precipitation periods. The concentrations of imidacloprid during the rainfall events are introduced into the model.

VS2DT uses aqueous phase concentrations, and only the initial total application concentration is known. The initial aqueous phase concentration is adjusted to meet the calculated initial total concentration in a 15 cm core. Site specific parameters such as meteorological data, soil parameters, and imidacloprid characteristics are used in the model. VS2DT will simulate 191 days using meteorological data from the treated watershed starting on February 19, 1996 and ending on August 28, 1996.

As with any model, VS2DT has problems which must be considered:

1) Aqueous phase concentrations are used as inputs for the model.
2) The evaporation boundary condition is treated differently from other boundaries where water leaves the domain; evaporating water is assumed to be solute free (No solute leaves the domain through evaporation.). Therefore, evaporation nodes may become concentrated as evaporation proceeds (Healy, 1990).
3) VS2DT does not account for losses due to uptake by plants (transpiration).
4) Preferential flow can not be simulated in VS2DT. Systems which exhibit preferential flow characteristics can not be accurately modeled.
5) VS2DT can only use a domain (grid) which has ≤ 36,000 nodes.
6) VS2DT assumes homogeneous and isotropic conditions within the defined soil textures.
7) Large nodal models with small discretization require fast computers with ample hard drive space and a great deal of memory.

Two conceptual models of different scales are used to simulate flow through the vadose zone. VS2DT has a *tilt* factor built into the code (Healy, 1990). At the top of the grid, the left side is A, while the right side is A'. When the tilt is used, A' is raised to create a downward slope from A' to A . (A is the pivot point.) Models 1 and 2 will have a 6% tilt.

Model 1

Model 1 is used to simulate the movement of imidacloprid from a single imidacloprid application through the top 15 cm and down to a single lysimeter (Figure 2). This model is a fragment of Model 2 and uses a finer grid (112 rows by 132 columns). The rows have a vertical height of 1 cm and the columns are 2.54 cm wide. The total height is 122 cm (4 ft) and the total horizontal distance is 335.3 cm (11 ft). Only two soil textures are used: loamy sand and sandy clay loam.

The imidacloprid aqueous concentration inputs will occur in 3 nodes representing a total volume of 45.7 cm^3 (6 cm x 7.62 cm x 1 cm). The observation nodes in Model 1 are used to record the initial concentrations in order to compare these results with the calculated values, and the lysimeter nodes are compared with the field data. In order to calibrate the model, the concentration of the observation nodes in the top 15 cm will be averaged and compared to the calculated total concentration in the upper 15 cm.

Model 2

Model 2 is used to simulate the movement of imidacloprid from the ground surface to the water table (Figure 2). The nodal

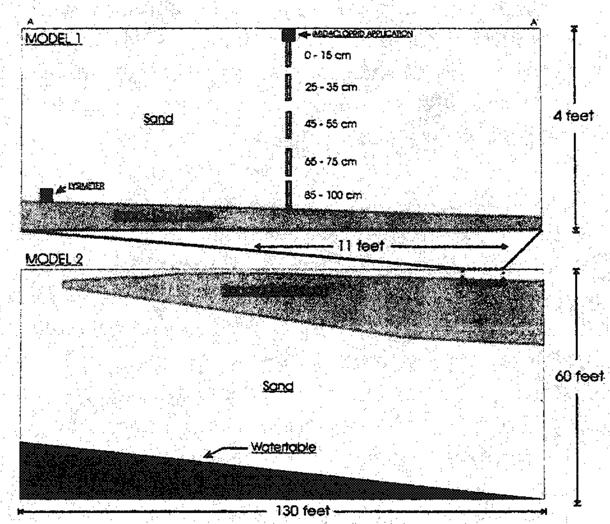

Figure 2. Conceptual models 1 and 2 used in VS2DT to simulate the movement of imidacloprid in a coastal plain setting. Both models are tilted 6% in VS2DT. (A' is raised 6 degrees.)

grid used in the model is 220 rows by 132 columns. The nodes for the first 111 rows have a vertical height of 1 cm. The next 68 rows have a vertical height of 7.62 cm (3 in), and the remaining 40 rows have a vertical height of 30.48 cm (1 ft). Horizontally, the 132 columns have a length of 30.48 cm (1 ft) per block. The total vertical distance is 60 ft to the water table and the total horizontal distance is 132 ft.

Three soil layers simulated are: loamy sand, sandy clay loam, and sand. At A', the loamy sand is 4 ft thick, the sandy clay loam layer is 17 ft thick, and the sand is 40 ft thick. At A, the loamy sand is 4 ft thick, and the sand is 57 ft thick.

Eight observation nodes are used to track the concentration of imidacloprid over time. The nodes are positioned in two columns: nodes consisting of all sand and nodes of sand-clay-sand down to the water table. This strategy allows the comparison of how imidacloprid behaves in the sand and in the sandy clay loam layers. The nodes closest to the water table for each column are used to estimate the concentration entering the groundwater.

Model 1 and 2 correlation

Model 1 is used to calibrate the predictions of VS2DT to the field data (both groundwater and lysimeter data) and the top 15 cm calculation. Once they agree, Model 2 is run using the same parameters as Model 1.

However, Model 2 has an initial concentration six times higher than Model 1 due to the difference in height of the application nodes.

VS2DT RESULTS

Calibration with calculated concentration

In order to accurately predict the movement of imidacloprid through the two models, the models must be calibrated to the calculated total concentration.

The concentration that both models predict is 2020 ppm in the top 15 cm. This value is consistent with the range from the calculations. After these calculations are verified for both models, the simulation is run for 191 days (~6 months), and the observation points at the lysimeter, water table and various points between are analyzed.

Lysimeters

The lysimeter concentrations predicted by VS2DT are below the detection limit (< 0.6 ppb). Based on these predictions, no imidacloprid reaches the lysimeters, and the concentration by day 191 averaged 10^{-28} ppb.

In the field however, lysimeter row LT13-18 was the only row of lysimeters to show measurable concentrations of imidacloprid. The lysimeters in this row are located in a distinctively different area from the other lysimeters. Lysimeters LT13-18 are positioned between large remnant stumps with extensive root systems which could cause preferential flow and could aid in the movement of solutes. The inputs for VS2DT do not account for this type of movement.

Discounting the model's predictions for row LT13-18 due to its inability to account for preferential flow, the model fits the field data by predicting that levels of imidacloprid in the lysimeters are far below detection limits.

Movement in a sand column versus sand-clay-sand column

Imidacloprid moves more quickly through the sand column than the sand-clay-sand (S-C-S) column. Detectable concentrations are predicted down to 220 cm (7.2 ft) in the sand column on the 191st day, but concentrations are below detection limits below that point. The S-C-S column shows that the concentration of the solute is severely retarded by the clay-enriched layer. Measurable concentrations are predicted within the upper 7.2 ft, but the nodes within the clay-enriched layer and below show concentrations far below detection limits. The solute travels approximately twice as fast and as far vertically in the sand column as in the S-C-S column.

Groundwater

The nodes at a depth of 57.1 ft (just above the water table) for both the sand and S-C-S columns, showed concentrations of imidacloprid below detection limits. This prediction agrees with the field data that shows that concentrations of imidacloprid in the groundwater are below detection limits.

CONCLUSIONS

Infiltration is the main agent of transport for imidacloprid. During rainfall events, imidacloprid desorbs from the application clay and increases the aqueous concentration in the soil-pore water. This relationship depends on the soil water content and amount of rainfall.

After rainfall events, evaporation dominates and the upper soil horizon dries. The aqueous concentration within the loamy sand nodes decreases during this period as the imidacloprid adsorbs to the soil.

Imidacloprid transport is different within the loamy sand and sandy clay loam layers. The insecticide travels more slowly through the clay-enriched layer than in the sandy layers. Computer simulations predict that imidacloprid will not reach the water table or lysimeters within 191 days following application.

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