ABSTRACT

One of the major factors contributing to surface water contamination in agricultural areas is the use of pesticides. The Soil and Water Assessment Tool (SWAT) is a hydrologic model capable of simulating the fate and transport of pesticides in an agricultural watershed. The SWAT model was used in this study to estimate stream flow and atrazine concentrations on a large-scale agricultural watershed in the midwestern USA.

The quality of water in agricultural watersheds has become an issue of major concern over the past several decades due to the transport of agricultural chemicals and pesticides to streams and aquifers through surface runoff and leaching. The movement of agricultural chemicals to surface and ground water systems is considered the main cause of nonpoint source (NPS) pollution throughout the USA (Yu et al., 2004).

Pesticides are commonly used in agricultural production systems throughout the world. Kalkhoff et al. (2003) identified the Corn Belt Region of the Midwest as one of the most intensive and productive agricultural regions in the world with nearly 80% of the country’s corn and soybean production and more than 100,000 Mg of pesticides applied to cropland annually. The use of pesticides in agricultural land has led to an increase in crop production; however, it has raised concerns about the adverse effects on the environment and human health. The use of pesticides may lead to contamination of surface and ground water (Louchart et al., 2001; Gaynor et al., 2002; Kalkhoff et al., 2003). Atrazine (2-chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine) is an inexpensive and effective herbicide that is widely used in corn production. In 2003, American farmers applied 25.3 million kilograms (55.6 million pounds) of atrazine to corn crops with the largest area of application being the Midwest Corn Belt Region (Kalkhoff et al., 2003). In recent years the concentration of atrazine in the surface waters of certain agricultural watersheds has been found to exceed 3 μg L⁻¹, the maximum contaminant level (MCL) established by the United States Environmental Protection Agency (USEPA, 2002).

The Cedar Creek Watershed (CCW), located in northeastern Indiana, is the largest tributary of the St. Joseph River, which supplies drinking water for approximately 250,000 people (SJRWI, 2004) in the city of Fort Wayne, Indiana. Concentrations of atrazine (3.7 to 10.0 μg L⁻¹) exceeding the safe drinking water standard were found in the tap water of Fort Wayne in 1995 (Cohen et al., 2003). Extensive treatment of the source water is required if the safe drinking water standard for atrazine is to be met. Approximately 76% of the St. Joseph River Watershed (SJRW) is under extensive corn production. It is believed that most of the pesticide found in streams comes from agricultural areas within the watershed due to corn production. Thus, effective watershed management requires a comprehensive understanding of hydrologic and chemical processes within the watershed. These relationships are frequently examined through simulation models and are used for assessing the effects of various management practices on water quality at the watershed scale.

Models serve as important tools for better understanding the hydrologic processes, developing new or improved management strategies, and in evaluating the risks and benefits of land use over various periods of time (Spruill et al., 2000). Spatially distributed hydrological models have important applications in the interpretation and prediction of the effects of land use change and climate variability on water quality, because they relate model parameters directly to physically observable land surface characteristics (Legesse et al., 2003). The Soil and Water Assessment Tool (SWAT) (Arnold et al., 1998) is a river basin-scale model that allows the user to divide a watershed into any number of subbasins. The SWAT

Abbreviations: CCW, Cedar Creek Watershed; ENS, Nash and Sutcliffe model efficiency coefficients; HRUs, hydrologic response units; R², coefficient of determination; SCS CN, soil conservation service runoff curve number; SWAT, Soil and Water Assessment Tool.
model can simulate and estimate pollution generation at the source and its movement from the source area to the receiving water body, providing flow and concentration histograms at various points in the watershed and entry points into the receiving water body.

The SWAT model has been used extensively within the USA, as well as internationally to study stream flow, sediment yields, and nutrient transport (Srinivasan et al., 1997; FitzHugh and Mackay, 2000). However, limited validation of pesticide simulation using SWAT has been attempted. To date, two studies have been reported in the literature using SWAT to simulate pesticide transport in northern central Indiana where the application of atrazine for weed control at the time of planting corn is common practice (Neitsch et al., 2002; Vasquez-Amabile et al., 2006). Due to the need for validating the SWAT model in predicting pesticide loads and the widespread environmental concerns associated with the use of pesticides, atrazine was selected to evaluate the accuracy of SWAT in predicting atrazine loads. Thus, the objectives of this study were to calibrate and validate the SWAT model for streamflow and atrazine concentration in the CCW and evaluate the use of the SWAT model for predicting atrazine levels in streams. Upon successful validation, SWAT could then be employed as a valuable tool for the Conservation Effects Assessment Project (CEAP) in simulating the impact of different management scenarios on the level of agricultural pollutants such as atrazine in the Midwest. The Conservation Effects Assessment Project is a nationwide project adopted by the U.S. Department of Agriculture (USDA) to quantify the environmental effects of conservation practices on water quality. The CCW has been designated as one of twelve benchmark watersheds participating in the 5-yr CEAP study.

**MATERIALS AND METHODS**

**Study Area Description**

The CCW is located within the St. Joseph River watershed in northeastern Indiana, 41°04′48″ to 41°56′24″ N and 84°52′12″ to 85°19′48″ W. The watershed drains two 11-digit hydrologic unit code (HUC) watersheds, the Upper (04100003080) and Lower Cedar (04100003090), covering approximately an area of 707 km² (Fig. 1). Topography of the watershed varies from rolling hills in Noble County to nearly level plains in Dekalb and Allen Counties with a maximum altitude above sea level of 326 m, and average land surface slope of 3%.

Soil types on the watershed were formed from compacted glacial till and fluvial materials. The predominate soil textures in the immediate Cedar Creek are silt loam, silty clay loam, and clay loam. The majority of the soils along Cedar Creek are the Morley-Blount and Eel-Martinsville-Genesee association. The Morley-Blount association usually occurs on the upland and indicates deep, moderately to poorly drained, nearly level to steep, medium-textured soils. The Eel-Martinsville-Genesee association consists of deep, moderately well drained, nearly level, and medium to moderately fine-textured soils on bottom lands and stream terraces (SJRWI, 2004).

The average annual precipitation in the watershed is approximately 900 mm. The average temperature during crop
growth seasons ranges from 10 to 23°C. Approximately 76% of the watershed area (SJRWI, 2004) is agriculture, 21% forested lands, and 3% urban. The majority of the agricultural lands are rotationally tiled predominantly with corn and soybeans, with lesser amounts of wheat and hay.

**Model Description**

The SWAT model was developed to simulate the hydrologic response of a large watershed with numerous subwatersheds. It is a spatially distributed, physically based hydrological model, which can operate on a daily time step as well as in annual steps for long-term simulation up to 100 yr. The SWAT model is a modification of the SWRRB (Simulator for Water Resources in Rural Basins) model that incorporates a new routing structure, flexibility in watershed configuration, irrigation water transfer, a lateral flow component, and a ground water component (Arnold et al., 1993). The SWAT model also incorporates shallow ground water flow, reach routing transmission losses, sediment transport, chemical transport, and transformations through streams, ponds, and reservoirs. The main purpose of the SWAT model is to predict the effect of different management practices on hydrology, sediment, and agricultural chemical yields in large ungaged watersheds.

Hydrologic processes simulated by the model include evapotranspiration (ET), infiltration, percolation losses, surface runoff, and lateral shallow aquifer and deep aquifer flow. The minimum weather inputs required by the model are maximum and minimum air temperature, and precipitation. Sediment yield is estimated using the Modified Universal Soil Loss Equation (MUSLE) developed by Williams (1975). Daily average soil temperature is simulated as a function of the maximum and minimum annual air temperatures, surface temperature, and drenching depth (Saleh et al., 2000).

The soil conservation service runoff curve number (SCS CN) (USDA, 1986) method or Green and Ampt (Green and Ampt, 1911) infiltration model is used to estimate surface runoff from precipitation. While the Green and Ampt method needs subdaily rainfall data, the SCS CN is adjusted according to moisture condition in the watershed. Evapotranspiration in the model (Arnold et al., 1993) is calculated by the Priestley-Taylor (Priestley and Taylor, 1972), Penman–Monteith method (Monteith, 1965), or Hargreaves methods (Hargreaves et al., 1985).

The SWAT model uses algorithms from GLEAMS (Ground Water Loading Effects on Agricultural Management Systems) (Leonard et al., 1987) to model pesticide movement and fate in land areas. The process is divided into three components: (i) pesticide processes in land areas, (ii) transport of pesticide from land areas to the stream network, and (iii) in-stream pesticide processes. Algorithms governing movement of soluble and sorbed forms of pesticide from land areas to the stream network were taken from EPIC model (Erosion–Productivity Impact Calculator) (Williams et al., 1985). The SWAT model incorporates a simple mass-balance method developed by Chapra (1997) to model the transformation and transport of pesticides in streams. The model assumes a well-mixed layer of water overlying a homogenous sediment layer. Only one pesticide can be routed through the stream network in a given simulation (Neitsch et al., 2001).

**Model Inputs for Cedar Creek Watershed**

The ArcView SWAT (AVSWAT2000) (DiLuzio et al., 2001) GIS interface was used for expediting model input and output. The elevation data (an important factor in the water dynamics throughout the watershed) was obtained from USGS at a map-scale of 1:24 000 quadrangle sheet data at 10-m elevation resolution to delineate the subwatershed slopes, stream network, and the watershed and subwatershed boundaries. The DEM (Digital Elevation Model) was projected to Universal Transverse Mercator (UTM) NAD83, Zone 16 for the state of Indiana. To obtain the proper stream path delineation, the 11-digit USGS boundaries of the Cedar Creek watershed, the upper and lower Cedar, were used as a mask and the stream delineation from the National Hydrograph Dataset (NHD) were overlain on the DEM and used to burn in the location of the streams in the watershed. A stream threshold minimum value of 650 ha was used to delineate 20 subbasins (Fig. 2). A USGS National Water Quality Assessment Program (NAWQA) water quality sampling station is co-located with the stream flow gauge station, thus the same delineation was used for both stream flow and atrazine calibration and validation.

In the SWAT model, Hydrologic Response Units (HRUs) are determined by the unique combination of land use and soils within each subbasin, whereby, the model establishes management practices. The thresholds for land use and soil used in this study were 5 and 10%, respectively, representing HRUs that are composed of at least 5% of land cover of the area in each subbasin, combined with soil types that occupy at least 10% of the area of that land cover (FitzHugh and Mackay, 2000). These thresholds values were selected to model the most significant cover types in the watershed, resulting in 259 HRUs, with an average of 13 per subbasin.

A description of land cover in the CCW was determined from the USDA National Agricultural Statistics Service (USDA-NASS, 2001), Indiana Cropland Data Layer. This land use is a raster, georeferenced, categorized land cover data layer produced using satellite imagery from the Thematic Mapper (TM) instrument on Landsat 5 and the Enhanced Thematic Mapper (ETM+) on Landsat 7. The imagery was collected between the dates of 29 Apr. 2001 and 5 Sept. 2001. The approximate scale is 1:100 000 with a ground resolution of 30 by 30 m.

Detailed information on soil type was needed to improve simulation results based on an increase or reduction in the number of HRUs (Mamillapalli, 1998). The SWAT2000 software can either accept the State Soils Geographic Database (STATSGO) spatial data, from the 1:250 000 scale underlying map, or the Soil Survey Geographic Database (SSURGO) from 1:12 000 to 1:63 000 scale from the USDA Natural Resources Conservation Service (USDA-NRCS, 2004). The SSURGO spatial data consists of county-level maps, metadata, and tables, which define the proportionate extent of the component soils and their properties for each map unit. For the counties intersecting the watershed, the SSURGO soil database is at a map scale of 1:12 000, and was created primarily for farm, landowner, township, or county natural resource planning and management. Due to the level of detailed information, the SSURGO soil database was used in this study. Forty-five soil SSURGO series are present in the CCW with Blount being dominant (25% of the watershed), followed by Morley (16%), Pewamo (16%), and Glynwood (10%).

Weather stations can either be located within the watershed or near the outlet. However, the farther the gauges are from the actual study site, the more likely the spatial variability of rainfall will affect the model results. The SWAT model is capable of generating climatic data for temperature, precipitation, wind, solar radiation, and relative humidity, or the data can be input. Daily precipitation and maximum and minimum air temperatures were obtained from the NOAA National Climate Data Center (NOAA-NCDC, 2004) for the Garrett Station with records from 1980 to 2003, and for the Waterloo Station with records from January 1997 to February 2003.
These two weather stations are located within the watershed and contained most of the dataset needed for the calibration and validation period of this study. Missing data for a given gauge were estimated from the Angola Station. Information on solar radiation, wind speed, and relative humidity were generated in SWAT.

For agricultural data, area-specific information on management activities was collected for the CCW during February 2005 to be used as input for the model. This information was provided by the St. Joseph River Watershed Initiative (SJRWI) project, and the Soil and Water Conservation Districts (SWCD) of Allen, Dekalb, and Noble Counties, which included the type of crops grown and the types of tillage practices, fertilizers, and pesticides used.

Corn and soybeans, the predominant crops in the watershed, are usually planted between late April and early May (Indiana Agricultural Statistics Service, 2003). Nitrogen fertilizer is primarily applied as anhydrous ammonia. Phosphorus is usually applied to corn and soybeans in granular form blended in various combinations with other nutrients. Atrazine-based herbicides are widely used to control weeds in corn and are surface-applied as a liquid. Glyphosate-tolerant corn hybrids are becoming increasingly popular in the area so the amount of atrazine applied is being reduced over time. The Soil and Water Conservation Districts of Dekalb County estimated that greater than 75% of all soybeans planted in the watershed are glyphosate-tolerant cultivars.

Conservation tillage has been widely adopted in the watershed. In Dekalb County 28% of all corn and 82% of all soybeans planted in 2004 were under a no-till system (IDNR, 2004). The tillage practices in Noble and Allen Counties differed only slightly from that in Dekalb County. However, the County SWCD offices regard tillage in the Cedar Creek portion of their county to be similar to that of neighboring Dekalb County. In general, all three counties exhibit similar agricultural trends within the watershed.

The timing, average rate, and number of atrazine applications were determined based on the seasonal progress of crop development and farm activities for northeastern Indiana reported by the NASS Agricultural Chemical Database. On average, the NASS reported 1.01 number of atrazine applications over a 7-yr period from 1996 to 2002 with a rate of 1.46 kg ha⁻¹ for northeastern Indiana (NASS, 2004). For the CCW, the timing of atrazine application was modified to account for the actual temporal application of pesticide in the watershed. Applications before, during, and after planting with an amount equal to the percentage of seasonal progress of crop development were used.

Tile drainage was assumed throughout the entire watershed for corn, soybeans, and winter wheat land cover. The tile drain area is considered to have an average depth of 0.8 m, which requires 48 h of drainage after a rain to reach field capacity, with a drain tile lag time of 2 h. The value for the SCS CN corresponding to each soil group and land use was used in the management. The SWAT model default values were used for the managements of forest, pasture, and urban areas.

Historical measured data for stream flow and atrazine concentration from the U.S. Geological Survey (USGS) were used to conduct the calibration and validation process. The calibration consisted of calibrating the stream flow for a 5-yr period from January 1997 to December 2001 at Gauge 04180000 (41°13′08″ N, 85°04′35″ W) Cedar Creek near Cedarville. A time period of 5 yr (from 1997 to 2001) was used for the calibration to ensure more precise parameter values. Validation was conducted for a 21-mo period from January 2002 to September 2003. Model calibration and validation for atrazine was then conducted with daily USGS National Water Water Quality Assessment (NAWQA) Sampling Station...
The stream flow data obtained from the USGS is composed of base flow and surface runoff. Base flow is the ground water contribution to stream flow, which needs to be separated out so that measured surface flow can be compared to simulated values. The base flow filter program (Arnold and Allen, 1999) was used to separate storm flow from base flow. The fraction of water yield contributed by base flow ranged between 44 and 60%. The base flow recession (ALPHA_BF), direct index of ground water flow response to changes in recharge, was 0.0171. The ground water delay (GW_DELAY) was 58 d. The ALPHA_BF and GW_DELAY were used in SWAT to account for subsurface water response.

The CCW dataset was set up to run on monthly and daily time steps for stream flow and atrazine concentration. The Penman–Monteith method was selected to compute ET to capture the effects of wind and relative humidity. The SCS CN was used to calculate surface runoff. A skewed normal distribution was assumed for rainfall distribution. The channel water routing needed to predict the changes in the magnitude of the peak and the corresponding stage of flow as a flood wave moves downstream was based on the Muskingum routing method (Cunge, 1969).

A warm-up period for the model is recommended to initialize and then approach reasonable starting values for model variables. The number of years to be considered depends on the objective of the study. Tolson and Shoemaker (2004) used a 2-yr warm-up period to provide reasonable initial channel sediment levels. Mamillapalli (1998) used a 5-yr warm-up period to minimize model initialization problems. A 10-yr period was found to reduce the influence of initial conditions on model results (Flay, 2001). The 15-yr water-balance simulation and a 3-yr warm-up period proved sufficient for model initialization in this study.

Model Evaluation Criteria

The accuracy of SWAT simulation results was determined by examination of the mean, standard deviation (STDEV), coefficient of determination ($R^2$), the root mean square error (RMSE), the Nash and Sutcliffe model efficiency coefficient ($E_{NS}$) (Nash and Sutcliffe, 1970), and the coefficient of residual mass (CRM) (Loague and Green, 1991). A comparison of both mean and STDEV indicates whether the frequency distribution of model results is similar to the measured frequency distribution. The $R^2$ value is an indicator of the strength of the linear relationship between the observed and simulated values. The RMSE is indicative of the error associated with estimated stream flow. The $E_{NS}$ simulation coefficient indicates how well the plot of observed vs. simulated values fits the 1:1 line. The $E_{NS}$ can range from −1 to 1, with 1 being a perfect agreement between the model and real data (Santhi et al., 2001). The CRM value can be positive or negative and gives the ideal value of zero when the observed and the predicted concentrations of the pesticide are equal. The RMSE, $E_{NS}$, and the CRM statistics are defined as:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (X_{oi} - X_{si})^2}$$  \hspace{1cm} [1]$$

$$E_{NS} = 1 - \frac{\sum_{i=1}^{n} (X_{oi} - X_{si})^2}{\sum_{i=1}^{n} (X_{si} - \bar{X}_{si})^2}$$  \hspace{1cm} [2]$$

Where $X_{oi}$ is the average measured value during the simulation period, $X_{si}$ is the simulated output on day $i$, and $X_{oi}$ is the observed data on day $i$.

The simulation results were considered to be good if $E_{NS} > 0.75$, and satisfactory if $0.36 < E_{NS} < 0.75$ (Van Liew and Garbrecht, 2003). A negative value of $E_{NS}$ indicates that the sum of squares of the difference between $X_{si}$ and $X_{oi}$ exceeds the sum of squares of the difference between $X_{si}$ and $X_{oi}$, which indicates that the observed data is a better predictor than the simulated data (Van Liew and Garbrecht, 2003).

Stream Flow and Atrazine Calibration

The SWAT model was calibrated according to the procedure recommended by Neitsch et al. (2002). The model was calibrated for stream flow using measured data from a USGS gauge located at the main outlet of the CCW near Cedarville, IN. Before calibration, an evaluation of the long-term water balance is recommended to ensure that the model simulations encompass periods with drier than average and wetter than average climatic conditions (Neitsch et al., 2002). A long-term simulation of SWAT for the CCW was performed over a 15-yr period from 1989 to 2004 to ensure that the model results were not biased toward one type of climatic condition, and to verify that the fractions of ground water and surface water contribution to stream flow were reasonable. In addition, model estimates of ET were found to be within the range of values representative of the area.

Calibration was implemented by changing one of the more sensitive parameters in the model and then observing the corresponding changes in simulated stream flow. In SWAT, the most sensitive parameters affecting flow were chosen as suggested in previous studies (Santhi et al., 2001; Van Liew and Garbrecht, 2003). These parameters are primarily the SCS CN, soil-available water capacity (SOL_AWC), and soil evaporation compensation factor (ESCO). The soil evaporation compensation factor is used to adjust the depth distribution for evaporation from the soil to account for the effect of capillary action, crust ing, and cracks. Calibration of these parameters is considered most critical since they may vary from one watershed to another even within the same geographical area. In this study, confidence is placed in a particular calibrated parameter set that produces a response most closely matching the measured data.

The model was run initially using the default flow parameters, with simulated monthly and daily stream flow being compared with measured data using the $R^2$ and the $E_{NS}$ statistics. The parameters that were adjusted during the model calibration are presented in Table 1. The value of any optimized parameter fell within a range of values considered to be pragmatic for calibration (Van Liew and Garbrecht, 2003). The SWAT original SCS CN default values for each land use were reduced by 10%, indicating that the CCW has better soil drainage for the type of soils, land use, and management practices specified than the assumed conditions in the model database. The ESCO value was reduced from 0.95 to 0.60 for cropland to allow for more evaporation from lower soil layers. The available soil water capacity was increased for cropland from 0.19 to 0.30. Other flow-related parameters that were modified included the Manning’s coefficient for overland flow ($OV_N$), the average slope length (SLSUBBBS), the maximum...
Table 1. Model input selected during calibration.

<table>
<thead>
<tr>
<th>SWAT Variable</th>
<th>Model processes description</th>
<th>Unit</th>
<th>Default</th>
<th>Value used</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Curve number for condition II</td>
<td></td>
<td>&lt;10%</td>
<td></td>
</tr>
<tr>
<td>ESCO</td>
<td>Soil evaporation compensation factor</td>
<td>0.95</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>SLSUBBBS</td>
<td>Average slope length m</td>
<td>121.0</td>
<td>150.0</td>
<td></td>
</tr>
<tr>
<td>OV_N</td>
<td>Manning’s a for overland flow storage</td>
<td>0.10</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>CANMX</td>
<td>Maximum canopy storage mm</td>
<td>0.0</td>
<td>10.0</td>
<td></td>
</tr>
<tr>
<td>SURLAG</td>
<td>Surface runoff lag time d</td>
<td>4.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>MSK_CO2</td>
<td>Impact of low flow storage time</td>
<td>3.50</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>Tile drain</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DDRAIN</td>
<td>Depth to subsurface drain mm</td>
<td>0.0</td>
<td>800.0</td>
<td></td>
</tr>
<tr>
<td>TDRAIN</td>
<td>Time to drain the soil to field capacity h</td>
<td>0.0</td>
<td>48.0</td>
<td></td>
</tr>
<tr>
<td>GDRRAIN</td>
<td>Drain tile lag time h</td>
<td>0.0</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>Soil</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOL_AWC</td>
<td>Soil-available water capacity mm</td>
<td>0.19</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>SOL_K</td>
<td>Soil hydraulic conductivity mm h^{-1}</td>
<td>5.79</td>
<td>10.0</td>
<td></td>
</tr>
<tr>
<td>Base flow</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GW_DELAY</td>
<td>Ground water delay d</td>
<td>31.0</td>
<td>58.0</td>
<td></td>
</tr>
<tr>
<td>ALPHA_BF</td>
<td>Alpha base flow factor d</td>
<td>0.048</td>
<td>0.0171</td>
<td></td>
</tr>
<tr>
<td>Pesticide</td>
<td></td>
<td></td>
<td>0.50</td>
<td>0.025</td>
</tr>
<tr>
<td>PERCOP</td>
<td>Partitioning of soluble pesticide between percolate and surface runoff</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

As in the case for stream flow, the model was run once using the default pesticide parameters with simulated monthly and daily atrazine concentrations being compared with measured data using the $R^2$ and the $E_{NS}$. Because a low model efficiency value was obtained using default values, the partitioning of soluble pesticide between percolate and surface runoff (PERCOP) was calibrated. A value of 0.025 for PERCOP was found to provide the best fit between measured and simulated atrazine data. Adjustments were also made in the timing of application based on crop stage and thereby, accounting for the actual temporal application of pesticide in the watershed. Since measured concentrations of atrazine are reported from late March to late September during each year, only data for those months were compared with the model simulation.

Model Validation

Once model parameters were optimized for calibration, model validation was performed based on monthly and daily USGS stream flow data, as well as for atrazine concentrations. The objective of the validation was to ensure that use of the calibrated parameters maintain a minimum deviation between measured and simulated values for a different simulation period and independent data set (January 2002 to September 2003), thus providing a reasonable measure of confidence in using the model. The same procedure was followed as in the calibration process in that the goodness-of-fit statistics were calculated to evaluate model performance and its ability to estimate stream flow for a time period other than that used for calibration.

RESULTS

Stream Flow and Atrazine Calibration

On an annual basis, the measured stream flow at the outlet of the CCW is estimated as 44 to 60% of base flow. In comparison, the simulated stream flow was estimated as 58 to 62% of base flow. The long-term water balance simulated by the model was similar to the long-term water balance for the northern portion of the state, as well as the long-term water balance recorded in the CCW (IDNR, 1980). Thus, the long-term water balance simulated by the model was considered to generate satisfactory predictions representative of the study area.

The measured and simulated stream flow are plotted in Table 2. Agreement between measured and simulated stream flow are shown by the $E_{NS}$ being 0.66 for both monthly and daily data sets. The $R^2$ values determined for monthly and daily calibration indicated a strong correlation between the measured and simulated stream flow. The $R^2$ value for monthly stream flow was greater than the value

Table 2. Monthly and daily calibration results for the Cedar Creek Watershed (CCW) from 1997 to 2001.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Time period</th>
<th>Observed</th>
<th>Simulated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>STDEV</td>
</tr>
<tr>
<td>Stream flow (m$^3$/s$^{-1}$)</td>
<td>Monthly</td>
<td>7.79</td>
<td>6.76</td>
</tr>
<tr>
<td></td>
<td>Daily</td>
<td>7.74</td>
<td>12.05</td>
</tr>
<tr>
<td>Atrazine (µg L$^{-1}$)</td>
<td>Monthly</td>
<td>1.15</td>
<td>1.35</td>
</tr>
<tr>
<td></td>
<td>Daily</td>
<td>1.42</td>
<td>1.90</td>
</tr>
</tbody>
</table>

† STDEV, standard deviation; RMSE, root mean square error; $E_{NS}$, Nash and Sutcliffe model efficiency; CRM, coefficient of residual mass.
obtained for daily stream flow, but still met the model criteria indicating that the model captured much of the measured stream flow trends.

A graph of simulated and measured stream flow calibration for the same period of time atrazine grab samples were collected is shown in Fig. 3. In general, the graphs show good agreement between measured and simulated stream flow. Measured and simulated peak stream flows occurred at the same location on the time scale. However, there are some events where the model does not agree well with measured stream flows. April and summer peak flows tend to be underestimated, and fall flows tend to be overestimated (Fig. 3). In general, the model usually underestimated the largest flow events.

On a monthly ($E_{NS} = 0.45$ and $R^2 = 0.51$) and daily ($E_{NS} = 0.45$ and $R^2 = 0.51$) basis model performance was lower for the first half of the year since most of the peak flow underestimations were observed during that period of the year. On the other hand, the monthly ($E_{NS} = 0.86$ and $R^2 = 0.89$) and daily ($E_{NS} = 0.74$ and $R^2 = 0.75$) statistics for the second half of the year showed good model performance. The average precipitation from April to September was approximately 588 mm while from October to March the rainfall amount was 396 mm, indicating that the model performed better during the drier period.

Values of $E_{NS}$ of 0.59 and 0.50 for monthly and daily atrazine simulations, respectively, were obtained indicating a satisfactory result (Table 2). The CRM values of 0.37 and 0.42 for monthly and daily simulations, respectively, show less difference between monthly and observed values than for daily values. The $R^2$ values for monthly and daily simulation indicated a strong correlation between the measured and SWAT-simulated atrazine concentration. The $R^2$ value for monthly atrazine (i.e., $R^2 = 0.66$) was higher than the value obtained for daily concentration (i.e., $R^2 = 0.57$). Overall, atrazine concentrations were underestimated in April, and from June to September for the 5-yr calibration period (Fig. 4). Overestimation was observed mostly in May, which corresponds to the period when most of the compound was applied, and when the highest peaks occurred in the measured data.

A graph of the simulated and measured daily atrazine is presented in Fig. 4. From the graph it can be observed that measured and simulated peak concentrations occurred simultaneously, and were present in surface water mainly during the months of May, June, and occasionally in July.

Stream Flow and Atrazine Validation

The model was validated for monthly and daily stream flow from January 2002 to September 2003. Again, model parameters from the calibration period were held constant for the validation. The results show that, overall, the model performed well for the independent data set with measured and simulated peak flow occurring at the same time, although there are differences in volume. A trend similar to the calibration results is observed during the validation period. As shown in Table 3, measured and simulated monthly and daily stream flow yielded $E_{NS}$ values of 0.56 and 0.51, respectively, indicating the model performed as well in the validation period as for the calibration period, although the validation efficiency values are somewhat lower than those obtained during the calibration period. As the time interval becomes shorter, model accuracy tends to decrease. Means for monthly and daily stream flow were also lower than those for measured data.

The monthly and daily stream flow patterns for the validation period were similar to the calibration period. The monthly $E_{NS}$ and $R^2$ values for the first half of the year were satisfactory ($E_{NS} = 0.38$ and $R^2 = 0.67$) while
for the second half of the year the values showed good performance ($E_{NS} = 0.85$ and $R^2 = 0.87$). A graph of the simulated and measured stream flow validation for the same period of time atrazine grab samples were collected is shown in Fig. 5. Possible explanations for discrepancies between model validation and calibration may be due to the period considered for validation, which was shorter than the period for calibration. However, the validation results indicate that once calibrated, the SWAT model can be quite effective in simulating and capturing stream flow dynamics on a large-scale agricultural watershed. Thus, the model would be a useful tool for studying the impact of various management practices on stream flow.

After calibration an independent set of data for atrazine concentration was used to validate the model. Statistical values were computed for monthly and daily validation estimates as shown in Table 3. The $E_{NS}$ values for monthly and daily atrazine yielded satisfactory results despite the fact that considerable variability was exhibited in the measured data. The CRM values of 0.23 and 0.26 for monthly and daily simulations, respectively, are very similar and indicate an overestimation by approximately 20% compared with measured data (Table 3). The $R^2$ values for monthly and daily validation indicate a strong correlation between the measured and SWAT-simulated atrazine concentrations. The $R^2$ values for monthly and daily varied slightly. The difference between mean measured and simulated values for monthly and daily was 22 and 26%, respectively, indicating that the model simulated less variability in the data during the validation.

A graph of the daily simulated and measured atrazine validation is shown in Fig. 6. Peak concentrations of atrazine in the creek, above the maximum contaminant level (MCL), followed a yearly pattern that is related to the timing of application simulated in the model and also for the first runoff event following application. Concentrations decreased through the summer and fall and are generally low or below detection until the following spring.

### DISCUSSION

For several decades pesticides have been widely used throughout the midwestern USA to control weeds in various types of farming systems. Due to its effectiveness and affordability, atrazine is one of the most commonly used pesticides in this region, as well as in areas of corn production throughout the world. Although the use of atrazine is beneficial in terms of potentially higher agricultural yields, the contamination of water quality is of great concern, particularly in water bodies such as the St. Joseph River that serve as a source for drinking water. Due to the limited validation of atrazine simulation using SWAT and the general environmental concern associated with the use of atrazine, the pesticide was selected to evaluate the accuracy of SWAT in predicting

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Observed</th>
<th>Simulated</th>
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<tbody>
<tr>
<td></td>
<td>Monthly</td>
<td>Daily</td>
</tr>
<tr>
<td>Stream flow ($m^3 s^{-1}$)</td>
<td>7.63</td>
<td>6.76</td>
</tr>
<tr>
<td>Atrazine ($\mu g L^{-1}$)</td>
<td>0.88</td>
<td>0.90</td>
</tr>
</tbody>
</table>

† STDEV, standard deviation; RMSE, root mean square error; $E_{NS}$, Nash and Sutcliffe model efficiency; CRM, coefficient of residual mass.
pesticide loads to streams in one of the major corn-producing areas of the country. Hence, once validated the model may be used as an effective tool in modeling different management scenarios aimed at preventing water contamination by atrazine, especially in watersheds with tile drainage systems.

To further evaluate the application of SWAT in the CCW, it is beneficial to contrast the results of this study with similar studies. Model efficiency coefficients in the literature consistently show higher values for monthly calibration vs. daily calibration values. Santhi et al. (2001) found monthly ENS values of 0.79 and 0.83 for 5-yr and 2-yr calibration periods, respectively; Saleh et al. (2000) reported monthly ENS values ranging from 0.65 to 0.99; Spruill et al. (2000) found for 1-yr period ENS values of 0.89 and 0.19 for monthly and daily stream flow, respectively. The ENS values for validation reported by Spruill et al. (2000) were always less than for calibration, while Santhi et al. (2001) reported greater ENS values for validation in some cases. In this study, however, ENS values were essentially the same for monthly and daily stream flow calibrations, and within the range of values reported in the literature even though the calibration and validation period of this study was much longer than that of other studies.

The improved performance of the model for the CCW study area may be attributed to the accuracy in simulating the soil and land use combinations. Mamillapalli (1998) obtained the best accuracy in stream flow simulation with the SWAT model using the same combination of soil and land use threshold used in our study. Furthermore, SWAT uses the curve number (SCS CN) technique to estimate stream flow, which largely depends on the soil and land use distribution. Although discretization of the CCW was not varied in this study, it is reasonable to assume that the number of subbasins simulated, in combination with an appropriate soil and land use threshold, resulted in improved model performance.
Possible explanations for model underestimation and overestimation of the stream flow may be attributed to some of the parameters in SWAT that govern flow through the shallow aquifer and deep aquifer simulated by the model, as well as the tile drainage routine used in SWAT. There is a considerable amount of uncertainty associated with estimating these parameters. Although SWAT has been greatly enhanced from its original version, further improvement in the tile drainage components should increase the accuracy in estimating stream flow and the atrazine load in watersheds with tile drains such as those throughout the Midwest.

The underestimation of the stream flow during summer may be more likely due to the lack of data on solar radiation and wind speed needed to estimate the potential ET by the Penman-Monteith method. The lack of available measured ET data in the study area to compare with model simulation results may lead to considerable uncertainty in ET estimates, thus greatly affecting the overall water balance. The overestimation of stream flow during fall and winter may be attributed to the difficulty in modeling snowmelt. Finally, the SCS CN curve number in SWAT represents an overall response of each HRU and does not account for near-stream saturation associated with excess runoff.

The availability of climate data plays an important role in model performance and accuracy. Spatial variability of precipitation data represents one of the major limitations in large scale hydrologic modeling (Arnold et al., 1998). Neitsch et al. (2002) calibrated the SWAT2000 model against 1-yr data and validated against 3-yr data in the Sugar Creek watershed located in the White River Basin draining 242 km² upstream from New Palestine, IN. They used data available from five weather stations located outside the watershed boundary. Calibration results for daily stream flow gave $R^2$ and ENS values of 0.59 and 0.47, respectively. The validation yielded $R^2$ and ENS values of 0.75 and 0.74, respectively. In a study conducted in the Little Washita River Experimental Watershed in Oklahoma, which drains an area of 610 km² with a total of 36 continuous precipitation-recording gauges, the $R^2$ and ENS values for monthly and daily stream flow for a 9-yr calibration period were 0.71 and 0.40, respectively (Van Liew and Garbrecht, 2003). Daily precipitation and temperature were recorded from twelve weather stations to use as input to calibrate the SWAT model for the Bosque River Watershed in Texas with an area of 4277 km². The monthly calibration results gave $R^2$ and ENS values ranging from 0.80 to 0.92 and 0.62 to 0.87, respectively (Santhi et al., 2001). Data from two weather stations were used to calibrate the SWAT model for the CCW from which precipitation must be distributed over all 20 subbasins. The majority of subbasins accessed data from the weather station located near the center of the watershed, which may misrepresent the distribution of rainfall over the entire watershed. Because SWAT runs on a daily time step using total daily precipitation and does not consider rainfall intensity, the volume of stream flow for some events may be considerably over or underestimated. Although the results given in this work meet the calibration criteria, the calibration may be improved if additional stream gauge and weather station data were available.

**SUMMARY AND CONCLUSIONS**

The hydrological and pesticide transport components of the SWAT model were tested on the 707 km² Cedar Creek Watershed (CCW) in northeastern Indiana. The predominant cropping system in the CCW is a corn-soybean rotation, which is typical in the midwestern USA. The hydrological components of SWAT were calibrated from January 1997 to December 2001 and validated from January 2002 to September 2003. For the calibration period, the Nash and Sutcliffe model efficiency ($E_{NS}$) between measured and simulated stream flows was 0.66 for monthly and daily intervals; whereas for the monthly and daily validation, $E_{NS}$ values were 0.56 and 0.51, respectively. Graphical examination showed that, once calibrated, the model adequately simulates the variations of observed stream flow data.

The pesticide component of SWAT was calibrated from January 1997 to December 2001, using measured atrazine concentration in surface water. Variations of atrazine concentration at the outlet of the watershed were well simulated by the model, with simulated concentrations in approximately the same range as measured values, and with peak concentrations occurring simultaneously. For the calibration period, $E_{NS}$ values between measured and simulated concentrations were 0.59 and 0.50 for monthly and daily intervals, respectively; whereas for the validation period, $E_{NS}$ values for monthly and daily simulation were 0.43 and 0.47, respectively. The highest peaks of atrazine concentrations were observed during May and June. Increased application rate during the critical period of crop development in the model caused an increase in atrazine concentration.

Overall, the SWAT model performed well in estimating stream flow and simulating (predicting) the general trends of monthly and daily atrazine concentrations in the CCW. Although we have discussed certain limitations of the model, when properly calibrated and validated, SWAT is suitable to evaluate the environmental effects of agricultural practices on water quality. Thus, the results of this study are significant in that they provide the basic modeling research, in terms of calibration and validation procedures, necessary for further use of SWAT as an assessment tool in evaluating the long-term effects of different management practices on atrazine transport in large, tile-drained agricultural watersheds in the Midwest region of the United States.

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**REFERENCES**


