1996

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Notes/Citation Information
Published in Transactions of the ASAE, v. 39, issue 4, p. 1367-1378.

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Digital Object Identifier (DOI)
https://doi.org/10.13031/2013.27628

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SIMULATION OF RUNOFF TRANSPORT OF ANIMAL MANURE CONSTITUENTS

Y. Wang, D. R. Edwards, T. C. Daniel, H. D. Scott

ABSTRACT. Runoff losses of land-applied animal manure constituents can adversely affect the quality of downstream waters. Reliable mathematical simulation models can help estimate runoff losses of animal manure constituents and identify management measures to reduce these losses. The objective of this study was to develop and calibrate an event-based simulation model to describe the runoff transport of solids (soil and manure particles) and nutrients (nitrogen and phosphorus) from areas treated with animal manure. The resulting model, consisting of linked hydrology, soil/manure transport, and nutrient transport components, is process-oriented and uses measurable parameters to the greatest degree possible. The three components of the model were calibrated sequentially (hydrology, soil/manure transport, and nutrient transport components) from areas treated with animal manure. The resulting model, consisting of linked hydrology, soil/manure transport, and nutrient transport components, is process-oriented and uses measurable parameters to the greatest degree possible. The three components of the model were calibrated sequentially (hydrology, soil/manure transport, and nutrient transport, in order) using data from plot-scale field experiments involving grassed plots treated with poultry litter. The calibrated parameter values were generally consistent with previously published values. Transport of total suspended solids, ammonia-nitrogen, dissolved phosphorus, and total phosphorus was well-predicted by the model. Transport of nitrate-nitrogen, however, was overpredicted by approximately an order of magnitude, while total Kjeldahl nitrogen transport was underpredicted by approximately an order of magnitude. Improvements in model structure (e.g., using different equations to describe the release of nitrate from the litter to the soil and assuming a significant proportion of organic nitrogen to be soluble) and parameter selection appear warranted to improve prediction of nitrate and total Kjeldahl nitrogen losses. Keywords. Nonpoint source pollution, Models, Runoff, Water quality.

Findings from field experiments have demonstrated that losses of nutrients, organic matter, and solids in runoff from areas treated with poultry manure are sensitive to the interval between application and first runoff event (Westerman and Overcash, 1980; Westerman et al., 1983; McLeod and Hegg, 1984; Edwards and Daniel, 1993a). The form of manure (i.e., solid vs. liquid or slurry), rate and method of manure application, and rainfall intensity are additional factors that can affect losses of various manure constituents (Edwards and Daniel, 1993a, b, c).

A variety of surface water quality models have been developed to simulate nonpoint source pollution from agricultural areas. In many of these models, processes of chemical transport from the soil surface to runoff are considerably simplified. Some models use extraction coefficients in describing chemical loadings to surface runoff and groundwater. The chemical losses estimated from this type of algorithm are calculated as products of average concentration in the soil water of the interaction zone, the extraction coefficient, and applicable water volume (infiltration volume for subsurface loss, runoff volume for surface loss). Complete mixing of chemicals within the interaction zone is commonly assumed (Frere et al., 1980; Young et al., 1985; Storm, 1987; Sharpley and Williams, 1990). Extensive studies related to groundwater quality modeling have been performed (Bear and Verruijt, 1987; Yaron et al., 1984; Leonard et al., 1988), some of which addressed nutrient transformation and transport processes associated with animal manure application (Ibrahim and Scott, 1989; Gilmour et al., 1987).

The overall objective of this study was to develop and calibrate a physically based, event-oriented, field-scale model to simulate runoff transport of solids (both soil and manure), nitrogen (N), and phosphorus (P) from areas...
treated with animal manure. Significant effort was devoted to theoretical descriptions of relevant physical processes to enhance tenability of the model and accuracy of the simulation results. The model has been written to be flexible in terms of input variables and management practices so that the user can assess the water quality impacts of factors such as manure application rates, timing of manure application, surface cover maintenance, and site characteristics. The model has been initially used to describe the situation of poultry litter applied to pasture shortly before a runoff-producing event. However, the model has been structured to facilitate adaptation to other manures and cover conditions by changing model parameters to reflect those different conditions.

The intent in developing this model was not to replace existing models that have the general capability of describing runoff quality impacts of animal manure application. There are several such models that are currently available, and there is ample documentation of these models’ effectiveness. The better-known of these models include the Agricultural Nonpoint Source (AGNPS) (Young et al., 1985) and Erosion/Productivity Impact Calculator (EPIC) (Sharpley and Williams, 1990) models. These models, like all others, were developed to be helpful in answering particular types of questions. The EPIC model, for instance, is well-suited to assessing long-term, field-scale trends in runoff quality in response to changing management practices, rainfall, and other variables. The AGNPS model, on the other hand, has the capability of incorporating spatially distributed data to assess water quality impacts of management practices on a watershed scale. The intended purpose of this model is to better understand and describe the physical and chemical processes by which manure application influences runoff quality. This purpose necessarily requires that the model be as physically based as possible. In terms of content and purpose, then, this model is most closely related to that reported by Khaleel et al. (1979a), who used physically based equations to describe the fate and transport of N in manure after land-application. The model reported in this article complements the model of Khaleel et al. (1979a) by incorporating a strong linkage between surface and subsurface water quality dynamics and by extending the applicability to soluble animal manure constituents.

MODEL DEVELOPMENT

The following paragraphs provide detailed descriptions of the model components, the equations and algorithms used, and assumptions incorporated into the model. In brief, the model consists of three major components: a hydrology component to relate runoff to rainfall and infiltration, a soil and manure transport component to model the detachment and transport of soil and manure particles, and a solute transport component to describe the transport of soluble N and P. Physically based equations are used as much as possible to reduce the need for calibration using observed data sets, although practical considerations do not allow this need to be eliminated.

The hydrology component is independent of the other two major model components, while the manure/soil transport and solute transport components require outputs from the hydrology component as their inputs. Transport of soil and manure particles is calculated directly in the manure/soil transport component. Transport of N and P is calculated from the outputs of both the manure/soil transport and the solute transport components. The specific model components and equations used in modeling transport of N and P depends on the particular nutrient form and the mode of transport taken as applicable to that form, as described later.

HYDROLOGY COMPONENT

The hydrology model component simulates overland flow during rainfall-runoff events. Since runoff is the transport agent for both soluble and particulate pollutants, simulation of hydrologic processes is the foundation of the following pollutant transport components. The hydrology component consists of continuity and momentum equations to describe overland flow as a function of space (x, one-dimensional) and time (t). The continuity equation used was:

\[
\frac{\partial q}{\partial x} + \frac{\partial y}{\partial t} = q_L \tag{1}
\]

where

- \( q \) = flow rate per unit width of the field (cm\(^3\)/s-cm)
- \( y \) = depth of the flow (cm)
- \( q_L \) = excess rainfall rate per unit area of the field (cm\(^3\)/s-cm\(^2\)).

The Mein and Larson (1973) version of the Green-Ampt (Green and Ampt, 1911) equation was used to calculate infiltration and thus \( q_L \). Manning's equation was used as the momentum equation to relate \( y \) to \( q \). The continuity and momentum equations were solved using a finite difference procedure that was developed by Li et al. (1975) specifically for application to the kinematic overland flow equations.

The outputs of the hydrology component include surface water ponding time, the time lag between the beginning of rainfall and onset of runoff, infiltration, and \( q \) and \( y \) as functions of \( x \) and \( t \). Major parameters required for this component include soil water content as a function of time and vertical distance from the soil surface, soil water potential at the wetting front, saturated hydraulic conductivity, and Manning's roughness coefficient for the soil surface. The soil water content distribution along the soil profile was determined using a groundwater and solute transport model developed by Scott and Ibrahim (Scott, 1989; Ibrahim and Scott, 1990). This model is a long-term simulation model that uses extensive data, including weather conditions, soil physical properties, crop growth status, and manure application parameters to describe the fates of land-applied poultry manure constituents.

SOIL AND MANURE TRANSPORT COMPONENT

The soil and manure transport component was based on results reported by Khaleel et al. (1979a) and Foster (1982). The simulated processes include rill and interrill detachment of both soil and poultry litter applied to the soil surface. The transport process is simulated using a sediment transport continuity equation, controlled by sediment transport capacities of individual particle size groups.

The continuity equation for sediment-litter transport is similar to that of the hydrology model in equation 1:
\[
\frac{\partial}{\partial x} (\gamma_{si} C_{si}) + \frac{\partial}{\partial t} (\gamma_{si} C_{si}) = D_i \quad (2)
\]

where

- \( \gamma_{si} \) = particle density for particle size i (g/cm\(^3\))
- \( C_{si} \) = sediment or manure concentration (cm\(^3/cm\(^3\)) in runoff
- \( D_i \) = detachment rate for particle size group i (g/s-cm\(^2\))

\( q \) and \( y \) = as defined in equation 1

The continuity equation was solved numerically by a finite difference method similar to that used for the hydrology component equations. The time and space increments for both the hydrology and sediment transport equations, and the upcoming solute transport equation, were held equal for consistency.

The sediment or manure discharge in equation 2 is controlled by corresponding transport capacities of respective individual particle size groups. The Yalin sediment transport equation was used in computing transport capacities for individual particle size classes (Yalin, 1963).

**SOLUTE TRANSPORT COMPONENT**

The equation used to describe solute transport was:

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} (uC) = \frac{\partial}{\partial x} \left( D_z \frac{\partial C}{\partial x} \right) + F(C) \quad (3)
\]

where

- \( C = C(x,t) \) = solute concentration in surface water flow (µg/cm\(^3\))
- \( u = u(x,t) \) = flow velocity of surface water flow (cm/s)
- \( D_z \) = dispersion coefficient in water (cm\(^2\)/s)
- \( F(C) \) = source/sink term

The source/sink term is described using Fick’s law as:

\[
F(C) = \frac{1}{y} \left( -vC + D_z \frac{\partial C}{\partial z} \right) = \frac{1}{y} \left( -vC + D_z \frac{C_0 - C}{\Delta z} \right) \quad (4)
\]

where

- \( F(C) \) = net solute mass flux to the runoff (µg/cm\(^3\)-s)
- \( v \) = infiltration velocity (cm/s)
- \( D_z \) = hydrodynamic dispersion coefficient in soil water (cm\(^2\)/s)
- \( \Delta z \) = depth of interaction zone (cm)
- \( C_0 \) = solute concentration at the bottom of interaction zone (µg/cm\(^3\))

The source/sink term \( F(C) \) describes the overall process by which soluble constituents move into runoff. Equation 4 accounts for advection (vC) and hydrodynamic dispersion (Dz \( \partial C/\partial z \)). The negative sign of the advection term indicates that the infiltrating water decreases the amount of solute at the soil surface that is potentially available for runoff transport. Solutes can thus enter runoff only through hydrodynamic dispersion, which includes the processes of molecular diffusion and mechanical dispersion. Molecular diffusion, as discussed later, is assumed negligible in comparison to mechanical dispersion, leaving mechanical dispersion as the only process through which solutes enter runoff. Furthermore, since the vertical component of infiltration velocity must be downward, longitudinal mechanical dispersion will not contribute to solute entry into runoff. Thus, solute entry into runoff can be thought of as occurring only through transverse mechanical dispersion and by virtue of a nonzero horizontal velocity component in the infiltrating water. Equation 4 admittedly does not describe transverse mechanical diffusion, and the hydrology model component does not account for lateral subsurface velocity components. The use of equation 4 thus represents a simplification of a situation that would otherwise require two-dimensional modeling of both flows and solute transport.

The boundary conditions used in equation 3 are:

\[
C(0,t) = C_{rain} \quad (5)
\]

\[
\frac{\partial C(x,t)}{\partial x} \bigg|_{x=L} = 0 \quad (6)
\]

and the initial condition is:

\[
C(x,0) = C_{rai} \quad (7)
\]

where \( C_{rain} \) is solute concentration in the rainfall water (µg/cm\(^3\)).

Equation 3 was solved numerically with using the Crank-Nicholson finite difference method. The values of the variables \( u \) and \( y \) are supplied from the hydrology model component. Values of \( v \) are also computed in the hydrology component as infiltration rate divided by soil porosity.

The solute concentration in the interaction zone, \( C_0 \), is a function of time, soil characteristics, animal manure application parameters, and weather conditions. As a rainfall event starts, the rainfall leaches the soluble constituents out of the manure into the soil profile. This process is simulated using the Scott-Ibrahim model, which accounts for nutrient transformations, plant uptake of nutrients, and interactions of solutes with soil. The main equation used in the Scott-Ibrahim model to describe these processes is similar to equation 3, but applied vertically.

**GENERAL ASSUMPTIONS**

The major assumptions contained in the model are:

1. Runoff occurs as diffuse overland flow, and the soluble constituents in the applied manure are released to the top layer of the soil profile. The mechanism of mass transport to runoff water is then controlled mainly by hydrodynamic dispersion. Therefore, equation 4 applies vertically.
2. Nutrient transformations are negligible during rainfall-runoff events.
3. Manure constituent concentration in runoff is uniform within the depth of surface water as a result of quick mixing within the shallow overland flow.
4. Adsorption-desorption activity is significant only in the soil profile and not in the runoff; thus, this activity is accounted for in the subsurface water and chemical transport component (Scott-Ibrahim model) and not the runoff solute transport component.
MODEL PARAMETERS

The hydrodynamic dispersion coefficient in surface water flow, \( D_x \), in equation 3 has been widely studied in the field of environmental hydraulics. Fischer et al. (1979) summarized values suggested for different hydraulic conditions. For turbulent flow with a depth of \( y \) down an inclined plane, the dispersion coefficient can be determined as:

\[
D_x = \frac{0.404}{\kappa^3} y \sqrt{g y S_0} \quad (8)
\]

where
\( D_x \) = hydrodynamic dispersion coefficient (cm\(^2\)/s)
\( g \) = gravitational acceleration (cm/s\(^2\))
\( S_0 \) = hydraulic gradient
\( \kappa \) = von Karman’s constant (dimensionless), taken as 0.4 for an inclined plane.

The hydrodynamic dispersion coefficient in soil water flow, \( D_z \), in equation 4, was described by Hornsby et al. (1973) and Van Genuchten et al. (1974) for flumeturon as a linear function of infiltration velocity:

\[
D_z = a + b v \quad (9)
\]

where \( v \) is the infiltration velocity from equation 4, and \( a \) and \( b \) are constants. The parameter \( a \) is referred to as the molecular diffusion coefficient. The parameter \( b \), known as the dispersivity, incorporates the effect of small scale variations in velocity magnitude and direction. In cases with appreciable infiltration velocities, the contribution of the molecular diffusion to the value of the hydrodynamic dispersion coefficient is quite small and can thus be neglected without significant error.

Ibrahim and Scott (1990) used equation 9 for ammonia-N (NH\(_3\)-N) and nitrate-N (NO\(_3\)-N) transport in the soil water. Equation 9 was used in this study in simulating transport of each solute (NH\(_3\)-N, NO\(_3\)-N, dissolved P). The dispersivity, \( b \), was optimized against observed chemical losses because of its high variability with respect to soil properties and hydraulic characteristics (Scott, 1993).

The depth of the top soil layer that controls mass transport to surface water (\( \Delta z \) in eq. 4), may be considered the effective depth of interaction. Studies devoted to quantifying the effective depth of interaction were reported by Sharpley (1985) and Ahuja et al. (1981). In this study, \( \Delta z \) was taken as a constant of 1 cm.

SIMULATION OF NITROGEN TRANSPORT

The N transport model component simulates NO\(_3\)-N, NH\(_3\)-N, and total Kjeldahl N (TKN) transport in runoff. Nitrate-N transport is simulated through direct use of the general solute transport component, equations 3 through 7, together with the Scott-Ibrahim model, which gives chemical concentration distributions within the soil profile. Total NH\(_3\)-N transport in runoff is simulated as the sum of dissolved NH\(_3\)-N and sediment-bound NH\(_3\)-N in mass or mean runoff concentration units:

\[
T_{N_{NH3}} = D_{NH3} + S_{NH3} \quad (10)
\]

where
\( T_{N_{NH3}} \) = total \( NH_3 \)-N transport in runoff
\( D_{NH3} \) = dissolved \( NH_3 \)-N
\( S_{NH3} \) = sediment-bound \( NH_3 \)-N

It is assumed that at the end of the lag between the beginnings of rainfall and runoff, during which concentrated NH\(_3\)-N from the applied manure enters the soil profile, the soil in the top layer of the profile will have equilibrated with the solute in terms of NH\(_3\)-N concentrations. Adsorption-desorption activity is thus considered negligible in the surface transport model. Therefore, \( D_{NH3} \), the dissolved portion of total NH\(_3\), is simulated by direct use of the general solute transport component with appropriate corresponding parameters.

The sediment-bound \( NH_3 \)-N is simulated using a Freundlich relationship:

\[
S = K C^{1/n} \quad (11)
\]

where
\( S \) = NH\(_3\)-N concentration on sediment (\( \mu g/g \))
\( C \) = total NH\(_3\)-N concentration (mg/L)
\( K \) and \( n \) = Freundlich constants

Because of a lack of directly applicable data, the adsorption isotherm constants for NH\(_3\)-N adsorption to sediment were taken as applicable to a clay soil (Malica Clay; Preul and Schroepfer, 1968) with values of 14 and 1.44 for \( K \) and \( n \), respectively. A linear Freundlich absorption relationship was used in the Scott-Ibrahim model for the parent soil used in this study (Captina silt loam) with \( n = 1 \), and \( K = 0.25 \) (Ibrahim, 1992).

Total Kjeldahl N loss in runoff is simulated as the sum of total NH\(_3\)-N and organic N in mass or mean runoff concentration units, assuming organic N is in particulate form:

\[
T_{KN} = T_{N_{NH3}} + N_{org} \quad (12)
\]

where \( N_{org} \), the organic N loss to runoff, is simulated as:

\[
N_{org} = f_{org} \times ER_{org} \times ML_{manure} \quad (13)
\]

where \( f_{org} \) is the weight fraction of organic N in the poultry litter, taken as 3.25% from previously published litter composition analyses (Edwards and Daniel, 1993a), \( ER_{org} \) is the enrichment ratio of the organic N as a result of selective erosion of poultry litter material, taken as 4 as reported by Novotny and Chesters (1981), and \( ML_{manure} \) is the mass loss of the eroded manure, which is calculated in the soil and manure transport component in this study.

SIMULATION OF PHOSPHORUS TRANSPORT

The phosphorous transport model component simulates dissolved P and total P as transported in solution and associated with sediment. Dissolved P is simulated by the general solute transport component, equations 3 through 7, together with the Scott-Ibrahim groundwater and solute transport model. The dissolved P is then equilibrated with the exchangeable P adsorbed on eroded soil particles.

Total P loss (TPP) is simulated as the sum of total exchangeable P (both adsorbed and dissolved portions) and particulate P from eroded manure:

\[
TPP = DP + PP = DP + PP_{ads} + PP_{org} \quad (14)
\]
where DP = mass loss from the solute transport component
PP = total particulate P loss
PP$_{ads}$ = a portion of the total PP loss, is the exchangeable P adsorbed on the sediment lost
PP$_{org}$ = organic portion of the total PP lost with eroded manure.

The exchangeable portion of the PP loss is simulated as:

\[
PP_{org} = Q^o \times ML_{sed}
\]  

(15)

where $Q^o$ is the P adsorption maximum, or P adsorption capacity on specific soils in \( \mu g/g \), and $ML_{sed}$ is the mass loss of sediment, in g, as computed in the soil and manure transport model component.

The organic portion of particulate P loss from the eroded manure $PP_{org}$ is simulated as a function of the mass loss of the applied manure:

\[
PP_{org} = f_{orgp} \times ER_{pp} \times ML_{manure}
\]  

(16)

where $f_{orgp}$ = fraction of particulate P of the applied manure
$ER_{pp}$ = enrichment ratio of the particulate P as a result of selective erosion
$ML_{manure}$ = mass loss of the applied manure, as simulated by the soil and manure transport component.

The main source of the P loss is most likely the applied manure for this situation (Edwards and Daniel, 1993a). As mentioned earlier, simulation of DP transport requires execution of the Scott-Ibrahim model for P concentration distribution through the soil profile. The model requires the fraction of soluble P in the manure applied as an input. This fraction was assumed to be the fraction of total P in the poultry litter in the form of ortho-P and was taken as 0.33 (ASAE, 1992). Therefore, the organic fraction of the total PP (in weight percentage of waste applied) can be determined as:

\[
f_{orgp} = f - f_{ortho}
\]  

(17)

where $f$ is the proportion of total P in the waste applied, and $f_{ortho}$ is the proportion of ortho-P (PO$_4$-P) in the applied poultry litter, or 0.33. The total P in poultry litter, $f$, was taken from manure composition analyses (Edwards and Daniel, 1993a).

The general solute transport component, equations 3 through 7, simulates DP transported from the top layer of the soil profile to runoff water. It is assumed that the DP will reach equilibrium with the exchangeable P adsorbed on the eroded soil particles by the time the water samples are chemically analyzed. A Langmuir isotherm relationship was used to perform the equilibrium calculation

\[
S = \frac{Q^o b C}{1 + b c}
\]  

(18)

where $S$ = exchangeable P adsorbed on the sediment (\( \mu g/g \))
$C$ = concentration in water (mg/L)

$Q^o$ = P adsorption maximum on sediment
$b$ = adsorption energy coefficient

Two sets of Langmuir isotherm coefficients were used in this study for parent soil and sediment. Values of the parameters $Q^o$ and $b$ were selected as 1 650 \( \mu g/g \) and 0.505 cm$^3$/\( \mu g \), respectively, for the sediment and 157 \( \mu g/g \) and 0.142 cm$^3$/\( \mu g \), respectively, for the parent soil, according to published estimates (Novotny and Chesters, 1981; Novotny et al., 1978).

It can be seen from equation 14 that the total PO$_4$-P loss to runoff consists of two components—DP from the solute transport model and exchangeable P lost with sediment. Before equilibrium, the mass balance is:

\[
PO_4 = DP + PP_{ads}
\]  

(19)

After equilibrium, the mass balance is:

\[
PO_4 = PO_{4(sol)} + PO_{4(ads)}
\]  

(20)

using

\[
S = \frac{PO_4 - PO_{4(sol)}}{ML_{sed}}
\]  

(21)

and

\[
C = \frac{PO_{4(sol)}}{R}
\]  

(22)

where $R$ is total runoff volume and the subscripts (sol) and (ads) denote in solution and adsorbed, respectively. Substituting equations 21 and 22 into the isotherm, equation 18 yields the P concentrations after equilibrium.

Performance of the equilibrium calculation might not be necessary when runoff P concentrations exceed 5 to 10 mg/L, because the P concentration on sediment quickly approaches $Q^o$, the adsorption maximum or the capacity. In that case, there should not be much difference between dissolved P concentration before and after the equilibrium.

**MODEL TESTING**

**SOURCE OF DATA**

The data used for model calibration were collected from rainfall simulator experiments conducted in late August, 1991 at the Main Agricultural Experiment Station of the University of Arkansas in Fayetteville (Edwards and Daniel, 1993a). Dimensions of the plots were 1.5 x 6.0 m with major axes oriented up and down slope. Each plot was graded to a uniform 5% slope, and the soil is Captina silt loam. A stand of fescue was established on the plots in the fall of 1990.

Poultry litter was applied to the plots 24 h before simulated rainfall. The experimental design was a 4 x 2 factorial with three replications. Poultry litter was applied at 0, 6, 12, and 24 mg/ha, corresponding to 0, 218, 435, and 870 kg N/ha. Rainfall was applied by the simulators at intensities of either 50 or 100 mm/h until runoff for 0.5 h had occurred on each plot.
The poultry litter was analyzed by the University of Arkansas Agricultural Services Laboratory for water content, total N, NH₃-N, NO₃-N, total P, pH, electrical conductivity, and other parameters. Runoff samples were collected during runoff, and flow-weighted composite samples were delivered to the University of Arkansas Water Quality Laboratory for analysis. The discrete runoff samples were used to derive hydrographs and total runoff volumes, and the flow-weighted composite samples were used for analysis of pollutant losses during runoff. Constituents analyzed in runoff include TKN, NH₃-N, NO₃-N, total P, dissolved P, COD, and total suspended solids (TSS).

**CALIBRATION OF MODEL PARAMETERS**

The accuracy of model output depends upon appropriate selection of model parameters. Efforts were made in this study to develop a theoretically tenable model and to use measurable parameters with physical significance. However, some of the parameters vary extensively, even within small geographical areas. For example, the saturated hydraulic conductivity of Captina silt loam as determined by laboratory measurements may have coefficients of variation as high as 200%, depending mostly upon macropore occurrence and distribution (Thiesse, 1984). Therefore, parameters with relatively high variance should be calibrated against observed data, if possible, before model application.

The optimization procedure used in this study was based on Bayesian statistical theory (Box and Tiao, 1973; Edwards, 1990). The objective function is in the form of the determinant of a matrix if multiple outputs are used for optimization, and in the form of a sum of squared residuals if only a single output is used. The method of search used in the optimization procedure is a direct search technique described by Monro (1971).

Since the hydrology model component is the driving force for the soil/manure transport and chemical transport components, and since both the hydrology and soil/manure transport components are the driving forces for the nutrient transport component, the three submodels were calibrated sequentially, beginning with the hydrology component, and then the soil/manure transport component, ending with the nutrient transport component.

In the hydrology component, the soil water potential at the wetting front was obtained from a soil water retention curve measured for Captina silt loam soil (Thiesse, 1984). The saturated hydraulic conductivity of the soil was also determined and reported by Thiesse (1984). Values of the saturated hydraulic conductivity, however, varied within a wide range; therefore, this parameter was determined by calibration.

The saturated hydraulic conductivity was optimized using two outputs—the time lag between beginning of rainfall and beginning of runoff, and total runoff volume. The optimized value of \( K_{sat} \) was found from:

\[
\hat{K}_{sat} = \min_{K_{sat}} \left( \frac{\sum t_i^2 \sum t_i R_i}{\sum t_i R_i \sum R_i^2} \right)
\]  
(23)

where
- \( K_{sat} \) = saturated hydraulic conductivity
- \( t_i \) = residual (difference between observed and predicted value) of time lag between beginnings of rainfall and runoff
- \( R_i \) = residual of runoff volume
- caret = optimized value

The runoff volumes and rainfall-runoff lag times are computed from the hydrology component according to the modified Green-Ampt equation, as described earlier, which includes \( K_{sat} \) as a variable. The size of the output residual matrix is \( 4 \times 2 \times 3 \), corresponding to the levels of litter application rates, levels of the rainfall intensities, and the number of replications.

In the soil and manure transport component, the manure/litter erodibility factor (used in computing TSS transport) was assumed to be a linear function of litter application rate; i.e.:

\[
K_m = a_0 + a_1 R_m
\]  
(24)

where
- \( K_m \) = erodibility factor
- \( R_m \) = manure application rate
- \( a_0 \) and \( a_1 \) = constants

In calibrating this equation, the intercept and slope of the linear function were optimized by minimizing the sum of squares of the TSS residuals, leading to an objective function of the form:

\[
(\hat{a}_0, \hat{a}_1) = \min_{a_0, a_1} \sum TSS_i^2
\]  
(25)

where \( a_0 \) and \( a_1 \) are the intercept and slope of the linear relationship between manure-litter erodibility factor and litter application rate, and the caret denotes the optimized value.

In the solute transport model component, the hydrodynamic dispersion coefficient \( D_z \) in the interaction zone was optimized, with NH₃-N mass transport residuals used to form the objective function. This led to a single parameter and single output optimization given as:

\[
(\hat{D}_z) = \min_{D_z} \sum (NH_3 - N_i)^2
\]  
(26)

where \( NH_3 - N_i \) is residual of total NH₃-N mass transport. It was assumed that \( D_z \), the hydrodynamic dispersion coefficient in soil water, is independent of types of chemical solutes. Thus this parameter was later used for P simulation without further optimization.

As noted previously, \( D_z \) was assumed to be a linear function of infiltration velocity. During the optimization, however, the intercept (molecular diffusion coefficient) was considered negligible. Thus only the slope of the relationship between \( D_z \) and infiltration velocity was optimized. This will be discussed in more detail in the following section.
RESULTS AND DISCUSSION

HYDROLOGY SIMULATION

Simulated runoff volumes were compared to the observed runoff volumes in terms of relative errors, i.e., runoff volume residuals divided by corresponding observed runoff volumes:

\[ R' = \frac{R_s - R}{R} \]  \hspace{1cm} (27)

where

- \( R' \) = relative residual of runoff volume (cm/cm)
- \( R \) = runoff volume from the field experiment (cm)
- \( R_s \) = simulated runoff volume (cm)

The comparison of observed versus predicted runoff volumes is shown in figure 1 for the two rainfall intensities (50 and 100 mm/h). The relative errors are well-distributed around the zero line. As stated in the model testing section of this article, the saturated hydraulic conductivity of the Captina soil \( K_{sat} \), was optimized, with residual time lags and runoff volumes contributing to the objective function. The value obtained by optimization was 1.65 cm/h, which compared well with laboratory values determined by Thiesse (1984) of 1.35 cm/h with a standard deviation of 1.87 cm/h.

It can be seen from figure 1 that runoff volumes for the high rainfall intensity were much better simulated, as relative runoff residuals of the high intensity are less than those for the low intensity. This phenomena has been recognized by many hydrologists and because variability in soil properties (which leads to local errors when using lumped parameter models) tends to be overwhelmed by rainfall intensity at higher intensities. The soil water characteristic curve may differ from plot to plot as a function of the soil structure. Manning's roughness coefficient may vary because of nonuniformity of surface cover, and saturation water content may also be different with small areas. However, these variations and their associated errors play a relatively less important role in predicting large runoff volumes than in predicting small runoff volumes.

The simulated hydrographs were also compared to those obtained from the field experiment (fig. 2a). The observed flow rates were higher than simulated and then fell below the simulated curves gradually. The use of a uniform initial soil water content may have been partly responsible for this finding. In the Green-Ampt infiltration equation, the total water potential consists of the distance to the wetting front, the depth of surface water, and the average suction at the wetting front. The suction at the wetting front varies with

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water content, and therefore changes the driving force of infiltration as the wetting front moves downwards.

**SOIL AND MANURE TRANSPORT SIMULATION**

The intercept and slope of the assumed linear response between soil-manure erodibility and application rate were optimized with the sum of TSS residuals forming the objective function. The simulated and observed yields of TSS are given in figure 2b. As demonstrated in figure 2b, the model was successfully calibrated for TSS prediction for the experimental conditions.

The linear relationship obtained between the erodibility of poultry litter and application rate was:

\[ K_m = 0.089 + 0.00071 R_m \]  

(28)

where \( K_m \) is poultry litter erodibility (mg-h/MJ-mm), and \( R_m \) is the litter application rate. A linear relationship between the two variables has been reported by other investigators (Edwards et al., 1994). Values of \( K_m \) varied from 0.012 to 0.026 (mg-h/MJ-mm), corresponding to application rates of 6 to 24 mg/ha of poultry litter. These values compared favorably with those reported by Khaleel et al. (1979b).

It should be noted that the TSS contains both soil and litter particles. Composition analysis of the TSS would help define the relative proportions of the two materials in the TSS. Another point is that the linear relationship of the erodibility factor was for poultry litter applied on the day before rainfall. Extension to different intervals between litter application and rainfall might require more variables in the function (e.g., time, temperature, air and soil surface moisture, and wind speed).

The successful simulation of soil and manure transport suggests that developing similar relationships between erodibility and application rate for each type of animal manure might further improve the simulations.

**NITROGEN TRANSPORT SIMULATIONS**

The optimum value of dispersivity (slope of the relationship between \( D_z \) and \( v \), eq. 9) was determined as 0.64 cm. The infiltration velocities during the field experiment were simulated to range from 0.01 to 0.03 cm/s. According to the linear relationship for the \( D_z \) in soil water flow, these velocities and the slope of 0.64 led to values of \( D_z \) from 0.006 to 0.021 cm²/s. These values coincided reasonably well with values reported by other researchers (Shamir and Harleman, 1967), 0.01 cm²/s. The optimum dispersivity value identified in this study was higher than those used by Shamir and Harleman (1967) and by Scott (1989), around 0.1 cm. This disparity might reflect that the velocity components responsible for the contributing transverse mechanical dispersion are lower than the infiltration velocities used in the model. The velocity discrepancy could in turn be a consequence of simplifying the two-dimensional mechanical dispersion process through the one-dimensional equation 4.

Simulated outputs of NH₃-N, NO₃-N, and TKN are compared with the observed results from the field experiments as reported by Edwards and Daniel (1993) in figures 3a through 3f. While the NH₃-N simulations matched favorably with the field observations, the NO₃-N losses were overestimated by an order of magnitude, and the TKN losses were underestimated by approximately the same proportion.

One of the possible factors leading to overestimated NO₃-N losses is the assumed pattern by which NO₃-N is leached out of the poultry litter by rainfall and runoff. In the Scott-Ibrahim model, NO₃-N release is assumed to occur at a constant rate over a 6-h rainfall event. Another potential factor is that, as a solute without ion-exchange with the soil matrix, the NO₃-N may be transported in the soil profile faster than other solutes with ion-exchange activities such as NH₃-N and PO₄-P. If this is true, then assumption (4) in the general solute transport component may not be valid, and different values of the hydrodynamic dispersion coefficient would be required.

Figure 3—Simulated and observed ammonia nitrogen (NH₃-N) mass losses (a) and runoff concentrations (b).
might need to be assigned for different solutes and the optimization of $D_0$ extended to each solute.

The underestimation of TKN may have been due to the assumption that all organic N is in particulate form and thus transported with manure and sediment. It might be more realistic to assume a soluble portion of organic N and to simulate some organic N transport similar to that of NH$_3$-N.

Phosphorous Transport Simulations

Total mass losses and mean runoff concentrations of dissolved P and total P were simulated using the same parameters optimized for NH$_3$-N simulation. The simulation results, as shown graphically in figures 4a through 4d, are very close to those from field experiments. The results of using parameters (primarily $D_0$) calibrated during the NH$_3$-N simulation for P simulation without further optimization enhances confidence in model reliability. This indicates that the solute transport model might be applicable with little modification to other soluble chemical components (e.g., pesticides).

The underestimation of P losses might be because the dispersion coefficient for P might be smaller than that for
NH₃-N, due to the strong affinity of P to soil particles. The ion-exchange of chemicals reduces the effective flux rate. This finding suggests that the dispersion coefficient should be calibrated to each soluble chemical with significant ion-exchange potential.

The total P losses were also underestimated slightly. Apparently, the underestimation of TP transport was largely due to the underestimation of particulate P transport. Since the adsorption maximum, Q₀ (for sediment), has been well studied, the area with the most potential to improve the simulation output may be the enrichment ratio of manure P during the selective runoff and erosion processes. The value of the enrichment ratio used in this study was 2.0, taken from Novotny and Chesters (1981).

The simulation results might also be improved if the composition analysis of the poultry litter included the ortho-P portion of total P. The value of this desorbable P portion used in this study was obtained from the ASAE standards (ASAE, 1992), and contains a coefficient of variation of around 30%.

**SUMMARY AND CONCLUSIONS**

An event-based model was developed to simulate sediment, poultry litter particle, and chemical transport in runoff from pasture areas treated with poultry litter. The

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Figure 4—(a) Simulated and observed dissolved phosphorus (DP) mass losses, (b) runoff concentrations, (c) total phosphorus (TP) mass losses, and (d) runoff concentrations.
model focuses on the theoretical background of the processes involved and uses measurable parameters to the greatest degree possible. The hydrology, soil and manure transport, and chemical transport components of the model were sequentially calibrated. All the calibrated parameters were confirmed to be reasonable by comparing the values optimized, and/or relationships assumed, with those found in published literature.

The simulated soil and manure transport in runoff matched favorably with the observed data. The assumed linear relationship between poultry litter erodibility and litter application rate resulted in values of the erodibility that compared favorably to those found in earlier studies.

Simulated NH$_3$-N losses in runoff compared fairly well with observed losses from the field experiment. The linear relationship of the hydrodynamic dispersion coefficient to infiltration velocity suggested in earlier studies was confirmed in this study by comparing their values. Losses of NO$_3$-N in runoff were overestimated by an order of magnitude. The causes might include the NO$_3$-N release pattern assumed and the use in this case of a dispersion coefficient that is applicable to a chemical with ion-exchange activity. Total Kjeldahl N losses were underestimated by about an order of magnitude. Assuming a significant portion of manure organic N to be in soluble form would probably improve the predictions of TKN transport.

The dissolved P losses were simulated successfully with the hydrodynamic dispersion coefficient calibrated from NH$_3$-N losses, which suggests possible extension of this model to other solutes such as pesticides. The total P losses were slightly underestimated. Suggestions to improve model predictions include composition tests of the manure and careful selection of appropriate enrichment ratios.

REFERENCES


