ERDC TN-SWWRP-09-2
January 2009

Simulation of Reactive Constituent Fate and Transport in Hydrologic Simulator GSSHA

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PURPOSE: The purpose of this System-Wide Water Resources Program (SWWRP) technical note is to describe the new fate and transport routines in the Gridded Surface Subsurface Hydrologic Analysis (GSSHA) model. GSSHA is a watershed analysis and management tool that has the ability to simulate the movement of water, sediment and associated constituents at fine-scale increments (< 100 m) for fine temporal scales (seconds) over watershed scale areas. The resulting tool is intended for calculating total maximum daily loads (TMDLs) (Downer and Byrd 2007), as well as analyzing project alternatives and evaluating best management practices (BMPs) designed to control contaminants. Because of the fine temporal and spatial scales that can be simulated, GSSHA has the ability to provide much greater information than commonly used TMDL models, such as Hydrological Simulation Program FORTRAN (HSPF) and Surface Water Analytical Tool (SWAT), which function on subwatershed scales and typically are used to provide information at daily, or coarser, intervals.

BACKGROUND: Receiving water bodies are harmed by the introduction of contaminants. The control of non-point contaminants may best be performed in upland areas near their source. GSSHA is a physics based, fully distributed, hydrologic and sediment transport model. The distributed nature of the model confers significant potential advantages over traditional lumped parameter and semi-distributed models for the analysis of non-point source pollutant fate and control.

The U.S. Department of Defense distributed hydrologic model Gridded Surface Subsurface Hydrologic Analysis Model (GSSHA) (Downer et al. 2006) has been developed to allow the physics based simulation of sediment erosion, transport, and deposition on a continuous basis (Downer and Byrd 2007). The methods described in Downer and Byrd (2007) for sediment transport are general formulations amenable to further development for reactive transport. Building upon this previous work, the capability to simulate constituent fate and transport has been added to the model. Though GSSHA is a coupled surface water/groundwater model, constituent fate and transport are only currently simulated in the surface water components of GSSHA: the soil column, the overland flow plane, and the stream channel network including reservoirs. Input loadings can be distributed on the overland flow plane either on the land surface or mixed in the soil column, included as point sources on the overland flow plane or in the channels, as precipitation, or as groundwater sources and/or sinks. Simple first order kinetics can be used to describe the reactions, or alternatively, full nutrient cycle kinetics can be simulated with the Nutrient Simulation Model (NSM) (Johnson and Gerald 2006). The methods employed are described in this technical note.

GSSHA is developed to simulate a watershed's response to meteorological inputs. Basic simulated physical processes include distributed rainfall, rainfall interception by vegetation, surface ponding and retention, infiltration, evapotranspiration, overland flow, streamflow, and lateral saturated groundwater flow. The model also simulates sub-surface drainage networks and includes seasonality effects related to snowfall/snowmelt and seasonal variability in plant transpiration and interception parameters. The model is intended for, and has been applied to the simulation of streamflow, flooding, soil moisture, sediment erosion and discharge.

The hydrologic/hydraulic components of GSSHA provide the information necessary to simulate contaminant transport. Key to simulating contaminants within a watershed, GSSHA provides the ability to link two-dimensional (2-D) overland flow transport to one-dimensional (1-D) transport in a stream network, as shown in Figure 1. The overland flow plane provides inputs to the channel network at each point where the channel network and overland flow plane coincide. Optionally, water and constituents can be allowed to spill back from the channel onto the overland flow plane.

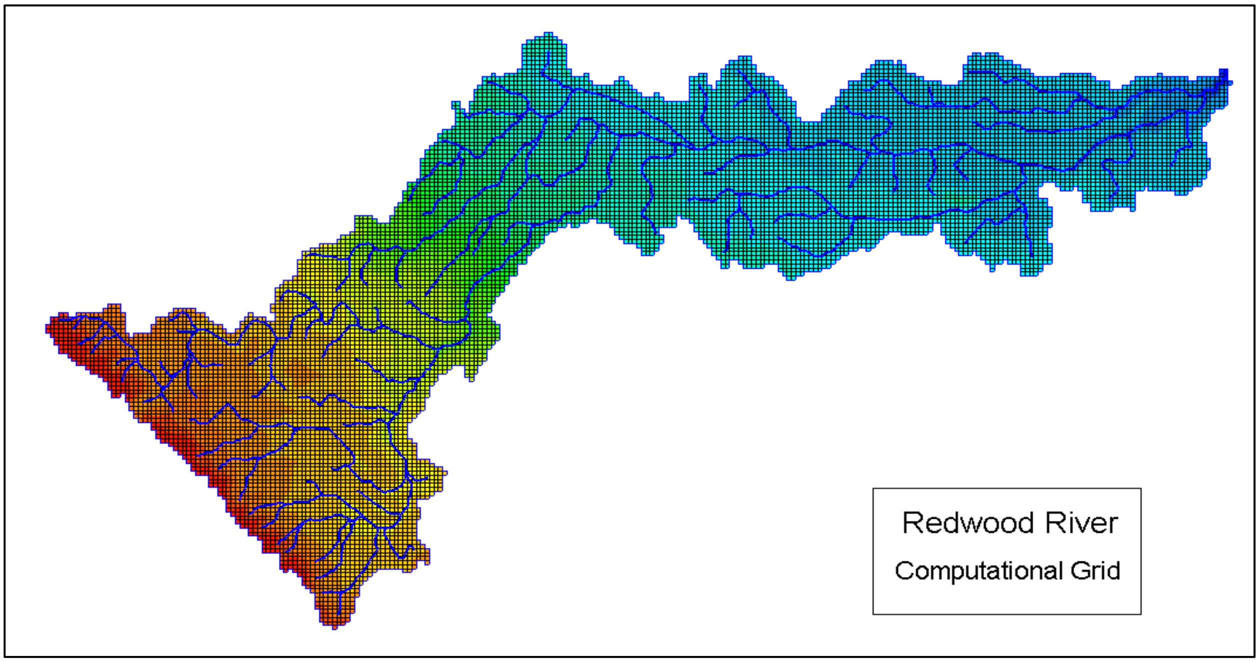

Figure 1. Representation of watershed, computational grid, and stream network in GSSHA.

Flow in both domains is described by the diffusive wave approximation of the Saint de Venant equations and solved using the finite volume technique. The finite volume method is inherently mass conserving and allows the simultaneous simulation of both wet and dry cells. The ability to simulate "dry bed" conditions is critical in the simulation of large, regional, watersheds as precipitation may occur preferentially within the study area and only sections of the watershed, or stream network, may be flowing at any given time.

The basic hydrologic model was expanded by Downer and Byrd (2007) to include the capability to realistically simulate both sediment and contaminants with physics based approaches. These approaches were validated at the Eau Galle watershed (Downer 2008). To extend the capability of the model for use in constituent transport, the model as described by Downer and Byrd (2007) has been modified to include the simulation of reactive constituents.

METHODOLOGY: Precipitation falling on the watershed may contain specified concentrations of contaminants. As rainfall accumulates on the land surface, contaminants on the land surface are dissolved and/or contaminants in the soil column diffuse into the overlying surface waters. Ponded surface water may infiltrate, providing a source of contaminants to the soil column, and/or move as surface runoff to adjacent cells. As water flows across the land surface, it is continuously affected by contaminated precipitation, exchange with contaminants on the land surface or in the soils, infiltration, and mixing with constituents in adjacent cells. Concentrations are also affected by decay and/or transformations. Because overland flow typically occurs for only brief periods of time, decay and transformation are generally minor compared to the physical processes affecting the constituents.

As overland flow reaches a stream channel, it is deposited into the channel and begins to move downstream, mixing with water and constituents already in the channel, and with water and constituents entering the channel at downstream locations. Additional point sources may enter the channel at any point. Interaction with the groundwater may represent either a source or a sink. As well as mixing with other sources, constituents in the channel also decay and/or transform. Decay and transformation are generally more important in the stream network, than on the overland flow plane. If the channel network includes reservoirs (Downer et al. 2008), significant decay and transformation can be expected to occur due to the long residence times in reservoirs.

At the end of a rainfall event, most or all of the overland flow plane will be dry. Any standing water will continue to infiltrate and evaporate. Constituent reactions will continue on the overland flow plane in any cells with remaining water. Baseflow may occur in channels. Groundwater provides a source of constituents to the channel if baseflow occurs. Reactions continue in the channel network as long as water is in the stream network. If reservoirs are included in the stream network, reactions continue in the reservoirs. In between events, constituents in the soil column may drain into the lower portions of the column and back to the groundwater. As the soil column dries due to drainage and evapotranspiration, the fraction of contaminants dissolved in the pore water versus that attached to the soil matrix changes. Reactions also continue for constituents in the pore water.

Although GSSHA is a fully integrated hydrologic model, water and associated constituents are associated with distinct domains which pass between domains as fluxes. For the current version of GSSHA (4.0) the domains including or affecting constituent transport are as follows:

1) Overland flow
2) Stream network
3) Reservoirs
4) Surface soils
5) Saturated groundwater

Currently the focus of the GSSHA model is the surface water transport of contaminants. Transport on the overland flow plane and within the channel network is treated with the general transport equations, as described in Downer and Byrd (2007). Reservoirs are treated as completely mixed reactors (CMR). Transport in the soils is due to advection between limited layers. The saturated groundwater is treated as having constant concentrations throughout the simulation. The details of how constituent transport is treated in each domain are described in the following section.

Overland Flow Transport. As described in Downer and Byrd (2007), contaminant transport on the overland flow plane is simulated by solving the advection diffusive equation (AD). Advection is the cell to cell movement of contaminants associated with water flow. Strictly speaking, diffusion is the molecular exchange that occurs due to concentration gradients. Practically speaking, the actual diffusion process is small, and the diffusion term is really a mixing term including several processes: physical dispersion, numerical dispersion, and molecular diffusion. The AD equation includes a source term to account for the various additions and subtraction of constituents as they move across the overland flow plane.

Sources and Sinks. Other than reactions, as described in the following paragraphs, the sources and sinks considered are as follows:

1) Addition by rainfall
2) Uptake from the soil surface
3) Exchange with soil
4) Infiltration
5) Exchange with channels
6) Exchange with groundwater
7) Addition by point sources
8) Exchange with reservoirs

Rainfall. The concentration (g m-3) of each constituent being simulated is constant throughout the simulation. Rainfall inputs are added directly to the overland flow plane, where they may either infiltrate, or pond and produce contaminated runoff.

Soil Surface. Contaminants on the overland flow plane can be considered in one of two ways. They can be considered to be laying on the soil surface, or they can be considered to be mixed in the soil column. The default is that contaminants are present on the soil surface. The amount of contaminants (Kg) is specified for each cell. Then, the mass transfer coefficient (*K*) (m s-1), specified for simple constituents, calculated for NSM, is used to move the contaminants into the overland flow based on the concentration deficit (solubility of the constituent and the concentration in solution). For simple constituents, these parameters are specified. For nutrients, these calculations are performed by the NSM. The mass flux (*F*) (g s-1) is computed as:

$$F = (C_{\max} - C_{ponded})KA \tag{1}$$

where:

$C_{\max}$ = maximum concentration (g m^{-3}) of the contaminant (solubility)
C_{ponded} = concentration of contaminant in the ponded surface water
A = the area of the computational grid cell (m^2).

Soil. Optionally, contaminants distributed on the overland flow plane at the beginning of the simulation may be mixed into the soil column. Currently, only the Green and Ampt with redistribution (GAR) model of infiltration (Ogden and Saghafian 1997) and the two layer soil moisture model (Downer 2007) can be used to simulate constituents in the soil column. When simulating constituents in the soil column, the mass of contaminants is distributed over a specified mixing depth in the soil column. Constituents in the soil partition between the soil matrix and the pore water based on the chemical properties, the soil properties, and the soil moisture. Constituent mass transfer into water ponded on the overland flow plane occurs due to the mass transfer coefficient (K) and the concentration difference between the soil pore water volume and the overland flow plane. As the concentration gradient may be in either direction, the flux may also be in either direction, i.e., the dispersive flux may be into the soil, acting as a sink for the overland plane. How constituents are treated in the soil column are discussed in detail later.

Infiltration. Some or all of the water ponded on the land surface may infiltrate, removing contaminants. Water that infiltrates is assumed to contain the same concentration of dissolved contaminants as the ponded water.

Channels. In general, the overland flow plane acts as the primary source of contaminants to the channel, which is a sink for the overland flow plane. For cases where overbank flooding occurs, the stream may overflow and add water, as well as constituents, back to the overland flow plane.

Groundwater. The overland flow plane interacts with the groundwater in two possible ways. If the groundwater table is high enough, water may spill out onto the overland flow plane as exfiltration. Without simulating soil contaminant transport, water spilling back on the overland flow plane has the specified groundwater concentration for that cell. If transport is being simulated in the soil column, the concentration of the exfiltrated water will be calculated as part of the soil constituent transport routine. Constituents seeping out of the soil column into the groundwater are accounted for but do not affect the static groundwater concentration for the cell.

Point Sources. Point sources may be input into any cell in the watershed. Point sources are defined by a constant discharge rate, Q (m^3 s^{-1}), and concentration, C (g m^{-3}), for each point source.

Reservoirs. Reservoirs in the channel network are also present within the overland flow plane (Downer et al. 2008). Water and constituents may be lost to a reservoir by either flowing into the reservoir, or by the reservoir rising and taking over the overland flow cell. Water and constituents may also flow from the reservoir back onto the overland flow plane. This results in a source for the overland cells adjacent to the rising reservoir.

Solution. Details of the numerical methods are discussed in Downer and Byrd (2007). The scheme is finite volume, so that fluxes are computed across cell faces in the x- and y-directions. The solution sweeps by rows and columns, alternating direction between subsequent calls.

Stream Network Transport. GSSHA computes values of water flow and depth within a user specified 1-D finite volume stream network. Solution of the diffusive wave approximation provides the discharge and cross-sectional area at fine space and time increments within the channel network. Typical stream nodes range in size from 30 to 200 m. Typical channel routing time-steps range from 5 to 30 sec.

This information is needed for the transport of constituents within the channel network using the general 1-D advection-dispersion equation in terms of the mass of constituent (M) equal to the concentration (C) multiplied by the volume (V) with constant dispersion. The details of the equations are described in Downer and Byrd (2007).

Sources and Sinks. For the channels, the following sources/sinks are considered in addition to chemical reactions.

1) Exchange with overland flow
2) Exchange with reservoirs
3) Exchange with groundwater
4) Point sources

Exchange with overland flow. As already described for overland flow, water from the overland flow plane is deposited in the stream network in overland grid cells that contain all or part of a stream node. If the channel spills back onto the overland flow plane, this is treated as a sink in the channel calculations.

Exchange with reservoirs. As described in Downer et al. (2008) stream networks may contain reservoirs. Water and constituents are lost to the channel in two ways. Water may flow into the reservoir from one or more upstream tributaries. The reservoir may also expand, taking stream nodes or entire reaches. When this occurs, any water and constituents in the overtaken stream node are removed from the channels and added to the reservoir. Discharges from reservoir outlets act as sources to the channel network.

Exchange with groundwater. Channel losses can be simulated whether or not the saturated groundwater surface is included in the simulation. When water seeps into the channel bottom, subsequent loss of constituents occurs as well. When the water table is included in the solution, as either static or varying, exchange can be in either direction. Concentration of constituents is specified for every cell in the groundwater domain. This concentration does not vary throughout the simulation. If flow is from the groundwater domain to the channel, water entering the channel is assumed to have the specified groundwater concentrations of constituents. Seepage from the channel to the groundwater is assumed to have the same concentration as the water in the channel node. Additions and subtractions to the groundwater are accounted for but do not affect the specified groundwater concentrations.

Point sources. Point sources may be input into any node in the stream network. Point sources can be defined as a constant discharge rate, Q ($m^3\ s^{-1}$), and concentration, C ($mg\ L^{-1}$), for each point source. Point sources may also vary in discharge and concentration over time. In this case the user specifies a time sequence of flows and concentrations for each point source.

Solution. Details of the numerical methods are presented in Downer and Byrd (2007). A finite volume scheme is employed, where fluxes are computed across the stream node faces in the longitudinal direction of flow. The solution employed is a predictor-corrector scheme.

- The original concentrations are used to estimate fluxes.
- Those fluxes are used to calculate intermediate concentrations.
- The intermediate concentrations are used to calculate intermediate fluxes.
- The original estimate of fluxes and the intermediate fluxes are averaged.
- Final concentrations are computed from the average fluxes.

In addition to the predictor-corrector scheme, the solution is iterative and proceeds until the maximum difference in concentrations in the channel network over successive iterations is less than $10^{-6}\ g\ m^{-3}$, or the maximum number of iterations is reached, currently set at 100 iterations. The predictor-corrector step is employed within each iteration.

Soil Column Transport. For simulations of transport in the soil column, infiltration must be simulated with the GAR infiltration model and soil moisture must be simulated with the simple soil moisture accounting routine. The simple soil moisture accounting routine (Downer 2007) allows the user to specify up to two soil layers for computation of soil moisture. Within these layers, downward soil water movement is due to gravity. If groundwater is being simulated, the groundwater may rise into the soil column, causing an upward flow of water in the soil column. Soil movement due to capillary pressure is not considered. Infiltration is a source to the top layer. Leakage from the bottom layer is considered a loss. Loss of water, but not constituents, also occurs due to ET, which is taken from both soil moisture layers.

Figure 2 shows the conceptual model of the soil column transport model. Downward fluxes (infiltration, gravity drainage, groundwater recharge) are shown on the left. Upward fluxes (exfiltration, upward groundwater flux) are shown on the right. Diffusive exchange occurs between the top soil layer and the surface water. Exchange between pore water and soil particles occurs in every layer, as does decay and transformations.

Distribution of constituents in soil column. When simulating constituents, a third constituent transport layer may be considered. Specification of this layer further divides the surface soil moisture layer. Any initial amount of constituents distributed on the overland flow plane is assumed to be mixed within this surface mixing layer. If this additional layer is not specified in the project file, the initial amount of contaminants is assumed to be evenly mixed over the top soil layer, and there will be only two layers in the soil transport model. If only one soil moisture layer is specified, then the initial amount of constituents is assumed to be mixed over this single layer, and transport is computed for one soil layer only.

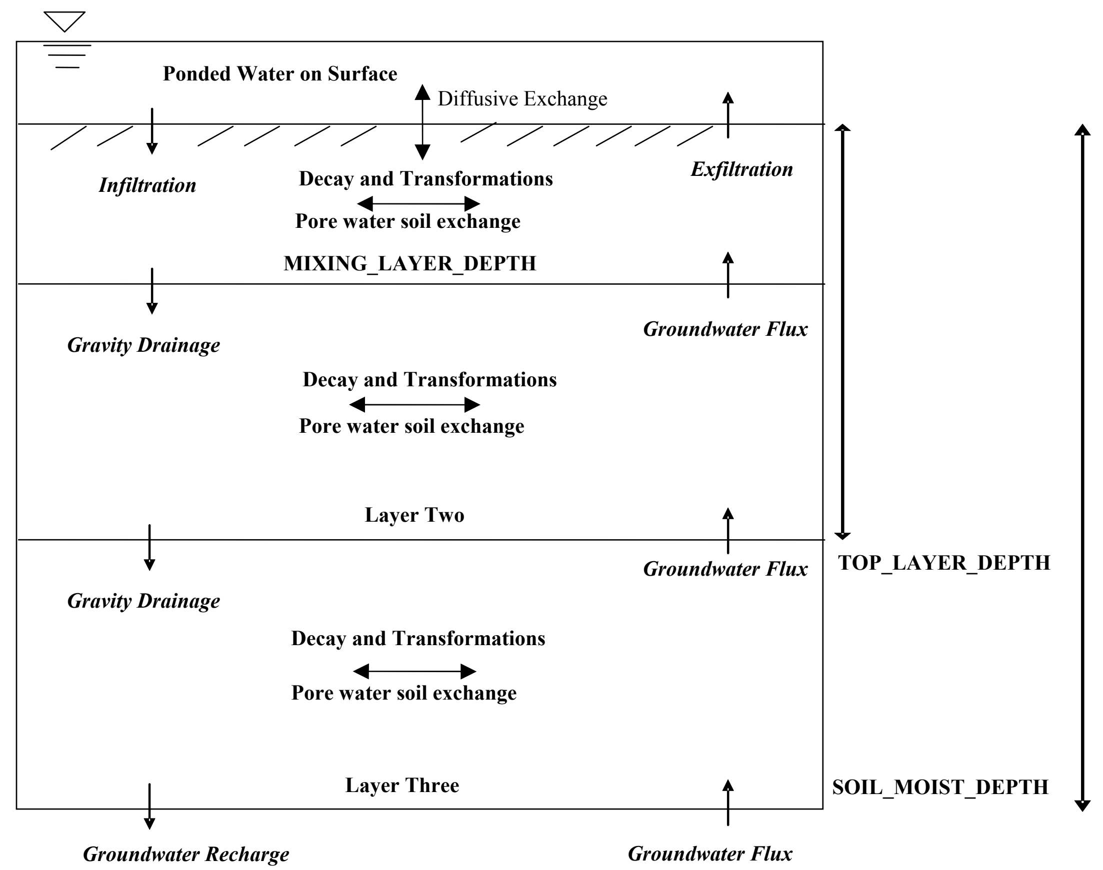

Figure 2. Soil column transport model.

Regardless of the total number of layers, the initial constituent loading is assumed to be mixed over the depth of the top layer. This mass of contaminants is distributed between an amount absorbed to the soil and dissolved in the pore water. The distribution is calculated based on the chemical distribution coefficient (K_d) (m^3 Kg^{-1}) and the soil moisture as described by Johnson and Gerald (2007). For the soils, the distribution between absorbed and dissolved is based on soil moisture (θ), and not porosity, as shown in Equation 2.

$$f_d = \frac{1}{\theta + K_d(1-\theta)\rho_s} \tag{2}$$

where:

f_d = fraction of the constituent dissolved in the soil layer
ρ_s = dry soil density (Kg m^{-3}). The concentration (g m^3) of constituent in the pore water (C_{pw}) is then:

$$C_{pw} = f_d MV \tag{3}$$

where:

M = total mass of constituent in the soil layer and V is the volume (m^3) of the soil layer:

$$V = \theta AD \tag{4}$$

where:

D = depth of the soil layer (m).

Exchange with surface water. During the simulation, infiltration acts as a source to the top layer. Advection of water transfers water and constituents to lower layers. Leakage from the bottom layer is a sink for that layer. The concentration of constituent in the advected water depends on the mass of contaminant in the layer, the soil moisture, and the distribution coefficient.

Mass exchange with water ponded on the land surface occurs due to the concentration gradient between the pore water in the top soil layer and the ponded water.

$$F = (C_{ponded} - C_{soil})KA \tag{5}$$

As can be seen in the equation, the direction of the flux is dependent of the relationship between the concentration of the surface water to the soil pore water volume. If the water on the land surface has a higher concentration than the soil pore water volume, the flux will be into the soil.

Interaction with groundwater. If the water table is being simulated, the water table may be present in any or all of the soil layers. If the water table is present in a layer, the amount of groundwater in that layer is considered in the calculation of soil moisture in the layer for the purposes of distributing the constituent between dissolved and attached fractions.

If exfiltration occurs, the groundwater is considered to come into the bottom layer, reach equilibrium condition in that layer and then move upward to the next layer, where it reaches equilibrium before being advected upward to the next layer, and ultimately to the land surface. The concentration reaching the land surface may not be the same as that specified for the groundwater in any given grid cell.

Reservoir Transport. Reservoirs in the stream network are treated separately from the channel network. Each reservoir is considered as a completely mixed reactor. As previously described, reservoirs interact with both the overland flow plane and the channel network. Reservoirs can also interact with the groundwater in the same manner as the channels, where the reservoir water and contaminants can seep to the groundwater, and the groundwater can supply water with static concentrations to reservoirs.

Groundwater Transport. GSSHA does not currently simulate fate and transport in the saturated groundwater. Whenever a water table is simulated in the GSSHA model, a concentration is specified for every grid cell in the watershed. Any flux from the groundwater to any other domain has the static constituent concentration of the groundwater cell that the flux occurs from.

Fluxes to and from the groundwater do not affect the groundwater concentrations. This simplified conceptualization of groundwater may not be adequate for simulating conditions where the groundwater exchange is significant and the groundwater concentrations vary with time over the period of the simulation.

Kinetic Reactions. Two types of reactive constituent transport are available in GSSHA. Constituents can be simulated as simple first order reactants with specified mass transfer rates from the soil and specified decay rates. For first order reactions, the mass decay rate (F) (g s^{-1}) is computed as:

$$F = KCV \tag{6}$$

where:

K = the decay rate (s^{-1})
C = the concentration (g m^{-3})
V = the volume (m^3) of water in the computational element.

The nutrient cycle can also be simulated with the Nutrient Simulation Model (NSM) Johnson and Gerald (2008). In either case, the overall simulation methods within the GSSHA model are the same. The selected kinetics, first order and/or NSM, provide the fluxes (F) to the different transport domains in GSSHA (overland, channels, soils). It is therefore possible to simulate nutrients as simple constituents, as well as simulating them with the full nutrient cycle. It is up to the user to determine the appropriate level of chemical kinetics for the problem to be solved. Specific kinetic routines are being developed for other contaminants of military concern (Johnson and Zhang, 2007) and others. In the future, these routines will be linked to GSSHA in a similar manner.

MODEL INPUT: As constituent fate and transport represent new components of the GSSHA model, the inputs are not covered in the original GSSHA users' manual (Downer and Ogden 2006). Updated information on the development of model input for constituent transport, as well as all other components of the GSSHA model, can be found on the GSSHA Wiki http://GSSHAwiki.com/index.php?title=Main_Page .

SUMMARY: The GSSHA model has been modified to allow the transport and fate of constituents in the surface water components of GSSHA: overland flow plane, stream network including reservoirs, and the soil column. The user specifies the number and properties of constituents to be simulated. The uptake of constituents from the overland flow plane and loss of materials in either the overland flow plane or stream network can simulated as first order reactions with specified rates, or as nutrients with uptake, decay, and transformation computed with the NSM model.

ADDITIONAL INFORMATION: This technical note was prepared by Charles W. Downer, Ph. D., P. E., research hydraulic engineer, Coastal and Hydraulics Laboratory, U.S. Army Engineer Research and Development Center. The study was conducted as an activity of the Regional Sediment Modeling and Management work unit of the System-Wide Water Resources Program (SWWRP). For information on SWWRP, please consult https://swwrp.usace.army.mil/

or contact the Program Manager, Dr. Steven L. Ashby: Steven.L.Ashby@usace.army.mil. This technical note should be cited as follows:

> Downer, C. W. 2009. *Simulation of reactive constituent fate and transport in hydrologic simulator GSSHA*. ERDC TN-SWWRP-09-2. Vicksburg, MS: U.S. Army Engineer Research and Development Center. https://swwrp.usace.army.mil/.

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