



Development of a Distributed Source Contaminant Transport Model for ARAMS

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INTRODUCTION: Given the complex nature of surface water and groundwater interaction, as well as the spatial nature of contaminant distribution, a distributed source contaminant transport model is needed to accurately account for the movement of water and contaminants through the various landscape media where more simplistic models are not applicable, or are homogeneous, which is not appropriate for the heterogeneous nature of distributed sources. This report will discuss the overland and channel flow formulations currently implemented within the Gridded Surface Sub-Surface Hydrologic Analysis (GSSHA) model. In addition, a detailed discussion of the contaminant fate and transport formulations for the overland, upper soil layer, and channel regimes will be presented. Finally, based upon training exercises, ongoing research, and proximity to Vicksburg, the Camp Shelby Training Area has been selected as the model validation site. Existing data and future data needs to support model calibration and validation will be discussed.

MODEL METHODOLOGY: In FY04, the flow components that can be found within the GSSHA model were evaluated. This section will detail the numerical flow formulations for overland and channel components and the proposed contaminant fate and transport formulations for the overland, upper soil zone layer, vadose zone, and channel regimes.

Overland Flow Methodology. Overland flow in *GSSHA* employs the same methods described for 1-D channel routing, except the calculations are made in two dimensions. Flow is routed in two orthogonal directions in each grid cell during each time step. The watershed boundary represents a no-flow boundary for the overland flow routing and when a grid cell lies on the watershed boundary, flow is not routed across the boundary. In *GSSHA*, $\Delta x = \Delta y$. Inter-cell fluxes in the x and y directions, p and q , respectively, are computed in cell ij from the depth d_{ij} at the n^{th} time level using the Manning equation for the head discharge relationship in the x and y directions, respectively, as

$$p_{ij}^n = \frac{1}{n} (d_{ij}^n)^{5/3} (S_{f_x}^n)^{1/2} \quad (1)$$

$$q_{ij}^n = \frac{1}{n} (d_{ij}^n)^{5/3} (S_{f_y}^n)^{1/2} \quad (2)$$

Depths in each cell are calculated at the $n+1$ time level based on the flows for each cell (Julien and Saghafian 1991):

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$$d_{ij}^{n+1} = d_{ij}^n + \frac{\Delta t}{\Delta x} (p_{i-1,j}^n + q_{i,j-1}^n - p_{ij}^n - q_{ij}^n) \quad (3)$$

In addition to this original formulation in the *CASC2D* model, two methods of solving the equations have been added, an alternating direction explicit scheme (*ADE*) and an *ADE* scheme with an additional predictor-corrector step (*ADEPC*) (Downer 2002, Downer et al. 2000). Both the *ADE* and *ADEPC* methods employ the up-gradient difference technique, Equation 40, for flows in the upstream direction (Downer 2002). Fluxes other than inter-cell fluxes, direct evaporation (DET), infiltration, and exfiltration, are accounted for before overland routing is computed.

In the *ADE* method, inter-cell flows are first calculated in the x direction according to Equation 1. Depths in each row are updated based on the flows in the x direction:

$$d_{ij}^{n+1/2} = d_{ij}^n + \frac{\Delta t}{\Delta x} (p_{i-1,j}^n - p_{ij}^n) \quad (4)$$

Inter-cell flows in the y direction are computed using the updated depths:

$$q_{ij}^{n+1/2} = \frac{1}{n} (d_{ij}^{n+1/2})^{5/3} (S_{f_y}^{n+1/2})^{1/2} \quad (5)$$

Depths in each column are updated based on the flows in the y direction:

$$d_{ij}^{n+1} = d_{ij}^{n+1/2} + \frac{\Delta t}{\Delta x} (q_{i,j-1}^{n+1/2} - q_{ij}^{n+1/2}) \quad (6)$$

With the *ADEPC* method, additional steps are added to improve accuracy and stability. As before, during each sweep, by rows or by columns, an estimate of heads is made based on the calculated flows, Equations 4 and 6. Next, using the updated depths, updated estimates of flow are computed at the $n+1$ time level

$$q_{ij}^{n+1} = \frac{1}{n} (d_{ij}^{n+1})^{5/3} (S_f^{n+1})^{1/2} \quad (7)$$

The original flows and the updated flows are then averaged to come up with an estimate of flows for the time step:

$$q_{ij}^{n+1/2} = (q_{ij}^n + q_{ij}^{n+1}) / 2.0 \quad (8)$$

These flows are then used to update the original depths, Equations 4 and 6. This procedure is essentially the MacCormack method (MacCormack 1969) except up-gradient differences are used in both the predictor and corrector steps. A similar method was successfully implemented by Wang and Hjelmfelt (1998).

Natural land surfaces contain micro-topography, small depressions, that retain water prior to runoff. The water held in the grid cell, or retention storage, never becomes direct runoff and can only be removed from the land surface as infiltration or direct evaporation. In certain regions, the retention storage can be significant. Retention storage is input as a depth (mm) in each grid cell.

Overland Contaminant Fate and Transport Methodology. The chemical transport module operating in parallel with the hydrological and sediment modeling components described above simulates the movement of chemicals. The chemicals applied in watersheds exist over the soil surface as well as below it. Chemicals may be deposited onto a watershed surface in different chemical forms, usually consisting of an aqueous phase, sorbed phases, and particles as:

- Dissolved phase in the overland flow.
- Dissolved phase in the upper soil layer.
- Adsorbed phase on suspended sediments in the overland flow.
- Adsorbed phase on soil particles in the upper soil layer.
- Separate particulate phase (not necessarily adsorbed to soil particles) in the overland flow.
- Separate particulate phase (not necessarily adsorbed to soil particles) in the upper soil layer.

During a rainfall event, chemicals can be surface transported while in the sorbed and particulate state (i.e., eroded) as well as while dissolved in runoff water. Chemical runoff includes dissolved, suspended particulate, and sediment sorbed chemical. Chemicals are moved by water and sediment, the movement of which, in turn, is dependent on climatic and watershed conditions. The processes governing chemical movement are much more complex than the runoff generation process. The complex process of chemical transport is affected by many factors such as advection, diffusion, adsorption-desorption, decay, and dissolution of the species. Kivva (2000) described two main processes determining chemical transport over land:

- Physical-chemical processes governing chemical distribution in the soil-water system, suspended sediment-surface water system, and surface water-upper soil layer system.
- Hydrological processes governing transport of water and suspended sediments, erosion and deposition processes.

The key kinetics processes are illustrated in Figure 1. The main physical exchange mechanisms between soil and surface water comprise soil erosion and deposition. These processes are controlled by hydraulic factors (e.g., raindrop energy, overland flow velocity, sediment transport capacity), and depend strongly on the sediment size and aggregation. Adsorption and desorption of chemicals by the suspended sediment and soil particles are the main chemical exchange processes, which are not always completely reversible. Any change in sorbed mass is accompanied by an immediate change in dissolved mass, and vice versa. Chemical transport on watersheds is influenced by all hydrological processes controlling the transport of water and sediment. Runoff formation begins after rain particles reach the surface. During the initial phase of runoff formation, rain energy liberates the soil particles, picks up the particulates and chemicals deposited on the surface, and dissolves the chemicals.

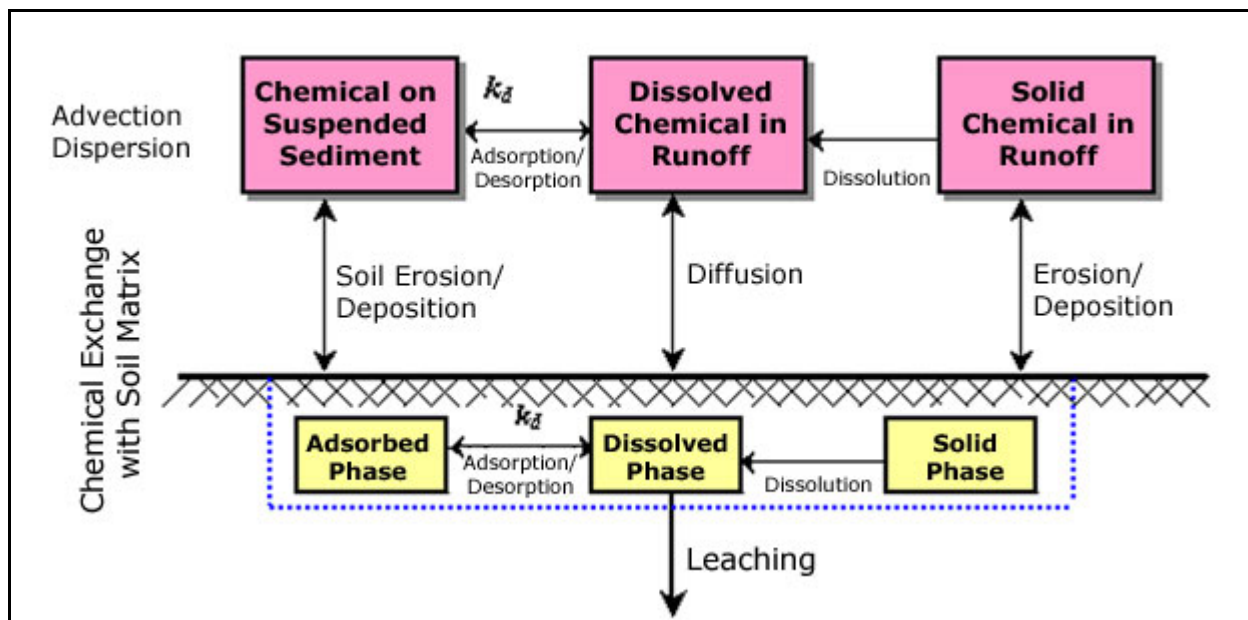


Figure 1. Schematic of overland chemical transport and transformation model

Several modeling efforts in the past have simulated the soil erosion process and chemical transport over land surfaces. But these models do not take into consideration the specification of the chemical transport and chemical interaction with sediments. There is no model available for simulating both soil erosion and chemical transport processes in conjunction with hydrologic processes. Explosive compound modeling at the watershed scale is still in its developmental stages. This overland module is able to simulate the detailed physical-chemical processes through which the chemicals of interest are transported from the soil surface to overland flow during runoff period.

Chemical kinetics processes and flux computations. The amount and form of chemicals within watersheds is determined by interaction of surface water with the upper soil layer, chemical transfer between surface water and suspended sediments, dissolution of the particulates (solute) into the water (solvent), and physical-chemical processes in the soil. The flux portion of chemical extraction into runoff is the most complex. Computing flux requires consideration of the following kinetic processes:

- Diffusion and turbulent transport of dissolved phase from soil pores to the runoff.
- Desorption from soil particles into the moving liquid boundary.
- Dissolution of stationary chemical particulates.
- Scouring of chemical particulates and their subsequent dissolution in the moving water.
- Entrainment in runoff while attached to suspended soil particles and their subsequent desorption in the moving water.

Adsorption-desorption. Chemical concentrations in water and on suspended sediments or solid particles are related through the distribution coefficient, i.e. the ratio of equilibrium concentrations of chemical in the respective solid and liquid phases. Distribution coefficient

values depend on sorption properties of the soil solid phase and chemical composition of water as well as properties and state of the chemical. When sorption kinetics are faster than advective transport rate, a distribution coefficient is simply employed to describe a linear equilibrium chemical concentration between the dissolved and adsorbed phase mass:

$$C_a^s = k_d^s C_d^s \quad (9)$$

$$C_a^r = k_d^r C_d^r \quad (10)$$

where:

- C_a^s = adsorbed chemical concentration on soil particles in upper soil layer (M/M)
- k_d^r, k_d^s = distribution coefficients for “water-suspended sediment” and “water-upper soil layer” systems (L^3/M), respectively
- C_d^s = dissolved chemical concentration in the upper soil layer (M/L^3)
- C_a^r = adsorbed chemical concentration on suspended sediment in the overland flow (M/M)
- C_d^r = dissolved chemical concentration in the overland flow (M/L^3)

When the local equilibrium assumption is not valid, the sorption process is often represented as a first-order reversible reaction:

$$\frac{\partial(C_a^r)}{\partial t} = k_s (k_d^r C_d^r - C_a^r) \quad (11)$$

$$\rho_b \frac{\partial(C_a^s)}{\partial t} = k_s (C_d^s - \frac{C_a^s}{k_d^s}) \quad (12)$$

where:

- ρ_b = bulk density of the soil (M/L^3)
- k_s = the first-order rate coefficient between the dissolved and sorbed phases for “water-suspended sediment” system ($1/T$)

Dissolved mass transfer. The chemical transfer between surface water and the upper soil layer is governed by both adsorption-desorption and diffusion processes. Dissolved chemical diffuses in either direction across the soil-water interface. From early experiments and calculations, it has been concluded that only a certain thin zone at the soil surface interacts with the rainfall and overland flow (Ahuja and Lehman 1983, Snyder and Woolhiser 1985). Effective depth of interaction is related to the degree of soil aggregation and it increases with soil slope, kinetic energy of raindrops, and rainfall intensity. Surface-applied or soil-incorporated chemicals are often transferred in significant quantities from soil to surface runoff as a result of rainfall. The transfer of dissolved chemicals from the soil solution to overland flow is a rate-limited process

proportional to the chemical concentration at the soil surface (Rivlin et al. 1997). It may be described as:

$$S_d = k_m (C_d^s - C_d^r) \quad (13)$$

where:

S_d = mass transfer rate of dissolved chemicals (M/L²/T)

k_m = dissolved mass transfer coefficient for water-upper soil layer (L/T)

The mass transfer coefficient relates solute flux across the soil surface interface to the difference in concentration between the soil solution at its surface and the runoff water. Using the film model theory, k was derived by the concentration gradient across the hydrodynamic boundary layer that separates the stagnant soil solution and the moving overland flow (Wallach et al. 1988, 1989).

Dissolution. Some chemicals may exist in separate solid phase and are not necessarily adsorbed to soil particles. Dissolution into water is a primary mechanism for the spread of solid chemical contamination. Once dissolved, the chemicals are available for transfer (i.e. adsorption) or transformation (i.e. biodegradation). The maximum aqueous concentration that the chemical can attain at a specific temperature if the water and solid phases remain in contact long enough is the solubility. Not only would modeling accuracy be improved by including solid chemical aqueous dissolution rates, but predicting hazard persistence and assessment of remediation alternatives affected by the dissolution of solid chemicals would be improved. One way to describe dissolution rate is using a first-order approximation of the dissolution process (Cussler 1997):

$$S_p = -\frac{D}{h} a(S - C) = -k_p a(S - C) \quad (14)$$

where:

S_p = mass dissolution rate of particulate solid chemical (M/T)

D = aqueous phase diffusion coefficient (L²/T)

h = boundary layer film thickness (L)

$D/h = k_p$ = also called the mass transfer coefficient (L²/T)

a = area available for mass transfer between the solid and liquid (L²)

S = solubility of the chemical (M/L³)

C = concentration in the bulk solution (M/L³)

For explosive compounds such as TNT, RDX, and HMX, dissolution rates have not been widely studied. The selection of dissolution model and rate greatly affect not only the predicted persistence of explosive compound sources but also their resulting concentrations in solution. Aqueous dissolution rate of explosive chemicals is affected by solid residue surface area, ambient water temperature, water mixing rate, and pH. Studies (Lynch et al. 2002) showed that

mixing rate and pH had much less effect on dissolution than surface area and temperature. Thus, the dissolution rate may be expressed as (Lynch et al. 2002):

$$S_p = a\beta e^{\theta T} \quad (15)$$

where:

T = water temperature ($^{\circ}\text{C}$)

β and θ = empirical coefficients for temperature effects

Erosion and chemical attachment. Many chemicals adsorb on to the soil particles, and are subsequently entrained into surface runoff as these particles are eroded by the moving water. This would require the inclusion of a surface erosion and sediment transport module. Since the wash-off involves chemicals in the soluble and particulate forms, both runoff and soil erosion processes are of importance. The runoff erosion process is governed by the processes involving raindrop-soil surface interaction as well as effects of anthropogenic activities. Surface erosion by overland flow is comprised of three processes. Detachment refers to the removal of particles from the flow bed. Transportation is the process by which eroded particles are carried within the flow and potentially deposited at downslope locations. The adsorbed chemical detachment due to soil erosion and sediment transport is computed by:

$$S_a = C_a^s(e_s + e_h), \quad e_h \geq 0 \quad (16)$$

$$S_a = C_a^s e_s + C_a^r e_h, \quad e_h < 0 \quad (17)$$

where:

S_a = adsorbed chemical mass rate with soil detachment ($\text{M/L}^2/\text{T}$)

e_s = soil splash erosion rate due to rainfall impact ($\text{M/L}^2/\text{T}$)

e_h = soil hydraulic erosion or deposition rate due to flowing water ($\text{M/L}^2/\text{T}$)

Overland chemical transport routing equations. Chemical transport is envisioned as two different transport phenomena: overland flow and the upper soil mixing zone. In the case of transport by overland flow, mixing is caused primarily by turbulence of overland flow and raindrop impact. The transport from the upper mixing zone is caused primarily by the mechanical mixing resulting from raindrop impact and the boundary turbulence of overlying overland flow (Singh 2002). The chemical transport by overland flow can take place in dissolved (soluble) form, adsorbed form, and in separate particulate form. Chemical transport in soluble form is a result of both the transfer of chemicals from soil water to the surface runoff water and desorption from the soil matrix and/or suspended sediments. The dissolved chemical on suspended sediments is a result of detachment of contaminated soil particles from the upper soil and/or adsorption from the soluble phase.

Water flow, chemical processes, and physical processes operate to transport, disperse, dissolve, adsorb, and transform the chemical contaminant. The chemical transport routing equation is

established based on the conservation of dissolved, adsorbed, and particulate chemical mass over a stationary control volume through which the fluid is flowing. The chemical reactions are modeled as a first-order process for which the rate of loss is proportional to the existing concentration to the first power. When diffusion effects are significant, the use of Fick's law of dispersion results in the appearance of additional terms.

Dissolved chemical transport by overland flow. Chemicals at or near the soil surface can be transformed to overland flow in solution form through desorption of adsorbed or absorbed chemicals from the soil in place; desorption of chemicals from eroded sediment, or adsorption of chemicals to eroded sediment; and dissolution of solid phase. Complete chemical transport in the aqueous phase by overland flow is described by the advection-dispersion equation:

$$\frac{\partial(hC_d^r)}{\partial t} + \frac{\partial(q_i C_d^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_d^r}{\partial x_j} \right) - fC_d^r + \Sigma S \quad (18)$$

where:

q_i = flow rate per unit width (L^2/T)

D_{ij} = coefficient of horizontal dispersion (L^2/T)

ΣS = chemical source/sink term representing the rate of change in dissolved mass due to biological and chemical reasons ($M/L^2/T$)

When the local equilibrium assumption is not valid in overland flow, combining Equations 16 and 17 with the Equations 11-15 leads to:

$$\begin{aligned} \frac{\partial(hC_d^r)}{\partial t} + \frac{\partial(q_i C_d^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_d^r}{\partial x_j} \right) - \\ fC_d^r - \lambda hC_d^r + k_m(C_d^s - C_d^r) - k_s hC_s(k_d^r C_d^r - C_a^r) + k_p(S - C_d^r) \end{aligned} \quad (19)$$

where λ is the lumped first-order decay rate for the dissolved phase in overland flow ($1/T$).

Transport of adsorbed chemical on suspended sediment by overland flow. Chemicals adsorb on to the soil particles, and are subsequently entrained into surface runoff as these particles are eroded by the moving water. Conservation of adsorbed chemical mass on suspended sediment is described by the following advection dispersion equations with the sink-source term describing soil erosion-deposition exchange processes:

$$\frac{\partial(hC_s C_a^r)}{\partial t} + \frac{\partial(q_i C_s C_a^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_s C_a^r}{\partial x_j} \right) + \Sigma S \quad (20)$$

where C_s is sediment concentration in water flow provided from the sediment module outputs (M/L^3).

When the local equilibrium assumption is not valid in overland flow, combining Equation 20 with Equations 11, 12, 16, and 17 leads to:

$$\frac{\partial(hC_s C_a^r)}{\partial t} + \frac{\partial(q_i C_s C_a^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_s C_a^r}{\partial x_j} \right) - \lambda hC_s C_a^r + C_a^s (e_s + e_h) + k_s hC_s (k_d^r C_d^r - C_a^r) \quad (21)$$

$$\frac{\partial(hC_s C_a^r)}{\partial t} + \frac{\partial(q_i C_s C_a^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_s C_a^r}{\partial x_j} \right) - \lambda hC_s C_a^r + (C_a^s e_s + C_a^r e_h) + hC_s (k_d^r C_d^r - C_a^r) \quad (22)$$

where λ is the lumped first-order decay rate for the adsorbed phase in overland flow (1/T).

Particulate solid chemical transport by overland flow. Separate particulate solid chemical transport is represented with a modification of the sediment transport equation and described by the advection-dispersion equations with the sink-source term describing solid chemical erosion-deposition exchange processes similar with the sediment transport:

$$\frac{\partial(hC_p^r)}{\partial t} + \frac{\partial(q_i C_p^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_p^r}{\partial x_j} \right) + \Sigma S \quad (23)$$

Combining Equation 23 with Equations 14 and 15 leads to:

$$\frac{\partial(hC_p^r)}{\partial t} + \frac{\partial(q_i C_p^r)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial C_p^r}{\partial x_j} \right) - \lambda hC_p^r + (e_s^p + e_h^p) - k_p (S - C_d^r) \quad (24)$$

where:

λ = lumped first-order decay rate for the solid phase in overland flow (1/T)

e_s^p = particulate chemical erosion rate due to rainfall impact (M/ L²/T)

e_h^p = particulate chemical hydraulic erosion or deposition rate due to flowing water (M/ L²/T)

e_s^p and e_h^p = calculated with similar splash and hydraulic soil erosion formulas.

Chemical transfer of upper soil layer. Assuming local equilibrium, dissolved, adsorbed and solid phase chemical transfer in the active upper soil layer are described by the following mass conservation equations:

Dissolved phase:

$$\Delta z \frac{\partial(\theta C_d^s)}{\partial t} = fC_d^r - fC_d^s - \lambda \Delta z \theta C_d^s - k_m(C_d^s - C_d^r) + k_p(S - C_d^s) \quad (25)$$

Adsorbed phase:

$$\rho_b \Delta z \frac{\partial C_a^s}{\partial t} = -\lambda \Delta z \rho_b C_a^s - C_a^s(e_s + e_h) \quad (26)$$

$$\rho_b \Delta z \frac{\partial C_a^s}{\partial t} = -\lambda \Delta z \rho_b C_a^s - C_a^s e_s - C_a^r e_h \quad (27)$$

Solid phase:

$$\Delta z \frac{\partial C_p^s}{\partial t} = -\lambda \Delta z C_p^s - (e_s^p + e_h^p) - k_p(S - C_d^s) \quad (28)$$

where:

Δz = depth of the upper soil layer (L)

θ = soil volumetric water content

λ = lumped first-order decay rate in soil (1/T).

Combining Equation 25 with Equations 26 and 27 leads to:

$$\Delta z \frac{\partial(\theta C_d^s + \rho_b C_a^s)}{\partial t} = fC_d^r - fC_d^s - \lambda \Delta z (\theta C_d^s + \rho_b C_a^s) - k_m(C_d^s - C_d^r) - C_a^s(e_s + e_h) + k_p(S - C_d^s) \quad (29)$$

$$\Delta z \frac{\partial(\theta C_d^s + \rho_b C_a^s)}{\partial t} = fC_d^r - fC_d^s - \lambda \Delta z (\theta C_d^s + \rho_b C_a^s) - k_m(C_d^s - C_d^r) - (C_a^s e_s + C_a^r e_h) + k_p(S - C_d^s) \quad (30)$$

For radioactive decay reaction, the first-order decay rate for the dissolved and sorbed phases are generally considered equal. However, for some forms of biodegradation, the two rates may differ. For overland transport, the longitudinal and transverse dispersion coefficients are given directly and the dispersion coefficients are determined as:

$$D_{xx} = D_{11} = D_L \frac{u_x^2}{u^2} + D_T \frac{u_y^2}{u^2} \quad (31)$$

$$D_{yy} = D_{22} = D_L \frac{u_x^2}{u^2} + D_T \frac{u_y^2}{u^2} \quad (32)$$

Channel Flow Methodology. *GSSHA* uses similar two-step explicit finite volume schemes to route water for both 1-D channels and 2-D overland flow, where flows are computed based on heads, and volumes are updated based on the computed flows. Compared with more sophisticated implicit finite difference and finite element schemes, the algorithm used in *GSSHA* is simple. The friction slope between one grid cell and its neighbors is calculated as the difference in water surface elevations divided by the grid size. Compared with the kinematic wave approach, this diffusive wave approach allows *GSSHA* to route water through pits or depressions, and regions of adverse slope. The Manning formula is used to relate flow depth to discharge. Use of the Manning formula implies that the flow is both turbulent and that the roughness is not dependent on flow depth. Neither of these assumptions may be valid on the overland flow plane. While being simple, the method is powerful because it allows calculations to proceed when only portions of the stream network or watershed are flowing. This is an important attribute, as rainfall may occur on only a portion of the watershed.

Explicit channel routing formulation. Inter-cell flows $Q_{i-1/2}$ and $Q_{i+1/2}$ (m^3s^{-1}) in the longitudinal x direction are computed from depths d at the n time level using the Manning equation for the head discharge relationship:

$$Q_{i+1/2}^n = \frac{1}{n} A_i^n (R_i^n)^{2/3} (S_{f_{i+1/2}}^n)^{1/2} \quad (33)$$

where:

n = roughness coefficient

A = area (m^2),

R = hydraulic radius

S_f = friction slope, calculated in the x direction as:

$$S_{f_{i+1/2}}^n = S_{o_{i+1/2}} - \frac{d_{i+1}^n - d_i^n}{\Delta x} \quad (34)$$

where S_{ox} is land surface slope in the x direction. If negative flow occurs (flow in the upstream direction), the head in the downstream cell is used to calculate the flow as:

$$Q_{i+1/2}^n = \frac{1}{n} A_{i+1}^n (R_{i+1}^n)^{2/3} (S_{f_{i+1/2}}^n)^{1/2} \quad (35)$$

Since the flow direction may change at any point in the stream, especially in ephemeral streams near the beginning of rainfall events, the flow direction is determined around each node and the locally upstream cell properties are used to compute the flow. This simple local determination of

the upstream cells prevents crashes in channels with adverse slopes when little or no water is present in the upstream cell. This method also allows better simulations of backwater effects.

Inter-node fluxes are used to calculate the volume V in each node as:

$$V_i^{n+1} = V_i^n + \Delta t(q_{lat}^{n+1} \Delta x + q_{recharge}^{n+1} \Delta x + Q_{i-1/2}^n - Q_{i+1/2}^n) \quad (36)$$

where:

$q_{lat} \text{ (m}^2\text{s}^{-1}\text{)}$ = amount of lateral inflow from the overland flow cells adjacent to the node

$q_{recharge} \text{ (m}^2\text{s}^{-1}\text{)}$ = exchange between the groundwater and channel

These new volumes are used to compute nodal values of A , d , and wetted perimeter at the $n+1$ time level. Calculations proceed from the upstream boundary to the downstream boundary.

Several modifications were made in implementing the channel routing scheme to accommodate groundwater/channel interactions. These modifications permit continuous interaction between channel nodes and the saturated groundwater cells. The channel routing scheme was modified to allow water to remain in the channel after channel routing ends, and for water to be present in the channel when channel routing begins. Because groundwater may discharge to the stream at any time, channel routing is initiated any time a minimum amount of water is in the channel network. If the channel routing scheme indicates there is no flow in the channel, channel routing is halted during periods outside precipitation events. Fluxes between the stream and the groundwater are still computed and stream volumes are adjusted without routing. If groundwater discharges to the stream, channel routing will resume, but at the groundwater time-step, which is typically larger than the channel routing time-step.

Because *GSSHA* uses a finite volume representation of channel flow, the standard stability criterion, Courant number < 1.0 , does not strictly apply. Maintaining stability is dependent on volume changes during each time-step. Experience with the scheme indicates that stability can be maintained with a time-step limitation that keeps the maximum Courant number everywhere in the network less than $1/6$. Groundwater and overbank fluxes can induce instability and additional controls in the channel routing scheme are added to further reduce instability. If the channel routing scheme becomes unstable (negative depth occurs in one or more cells), despite the more restrictive control on the Courant number, the time-step is reduced and the channel routing calculations are repeated. The channel routing time-step may be automatically reduced to a value as low as $1/1000$ of a second. Allowing the time-step to become very small during periods of sharp transition allows a larger overall model time-step to be used. For each call of the channel routing function, the overall model time-step is used as the beginning channel routing time-step. The time-step is only reduced when the stability controls are activated, and then only for that call of the channel routing routine.

The upstream boundary condition in each first-order link is a no-flow condition. The default watershed outlet condition is normal flow, calculated using the channel slope at the watershed outlet. The downstream boundary condition can also be a specified head. When the head boundary is specified, the depth at the outlet remains at the specified depth for the entire

simulation period. Flows entering the outlet cell exit at the same rate. The head boundary condition is desirable when the condition at the outlet of the basin is a known head instead of normal depth. This might occur when the basin empties into a larger water body such as a river, pond, or lake, or when a hydraulic structure is near the watershed outlet. The up-gradient method of computing inter-node discharges allows the head boundary condition influence to propagate upstream.

The default for the explicit scheme is to start simulations from the dry bed condition. A new feature for the explicit channel routing scheme is the ability to save water surface profiles and flows from one simulation and use them as the initial condition of another simulation.

Channel Contaminant Fate and Transport Methodology. Water quality changes in channels and streams within a watershed are due to physical transport and exchange processes, biological, chemical, biochemical, and physical conversion processes. A basic principle of stream water quality models is the conservation of mass. This principle requires that the mass of each water quality constituent being investigated must be accounted for in one way or another. A general governing equation of water quality models in the stream can be represented conceptually as:

$$\frac{\partial C}{\partial t} = [Dispersion] + [Advection] + [Reaction / Interaction] + [Source / Sink] \quad (37)$$

This equation represents the three major water quality processes: transport, loading, and transformation. The 1-D model is taken as the basic model in GSSHA to provide the chemical transport simulation in the stream network. The modeling approaches here consider transport and fate of the chemical in all three different phases - solid phase, dissolved phase, and adsorbed chemicals on suspended sediments in stream water. Including bed sediments and interaction among water, chemicals, and sediment components adds new terms to the model. Chemicals not lost through decay or volatilization may settle to the bottom sediments. Within the sediments, chemicals are subject to decay and burial. The main processes governing the chemical transport in stream systems are presented in Figure 2. The chemicals in streams are transported by the water flow (advection processes) with the simultaneous influence of the turbulent diffusion processes. The chemicals can interact with the suspended sediments and bottom bed depositions. Chemical transfer between the stream water and the suspended sediment is described by the adsorption-desorption processes. The transfer between the stream water and the upper layer of the bottom deposition is under the influence of adsorption-desorption and diffusion processes. The sedimentation of contaminated suspended sediments and bottom erosion are also important pathways of the “water column-bottom” chemical exchange. Within the water and sediment layer, the chemicals in three phases are subject to the decay/degradation process. The stream chemical simulation module is driven by the hydraulic module, which describes water, suspended sediment, and bottom dynamics.

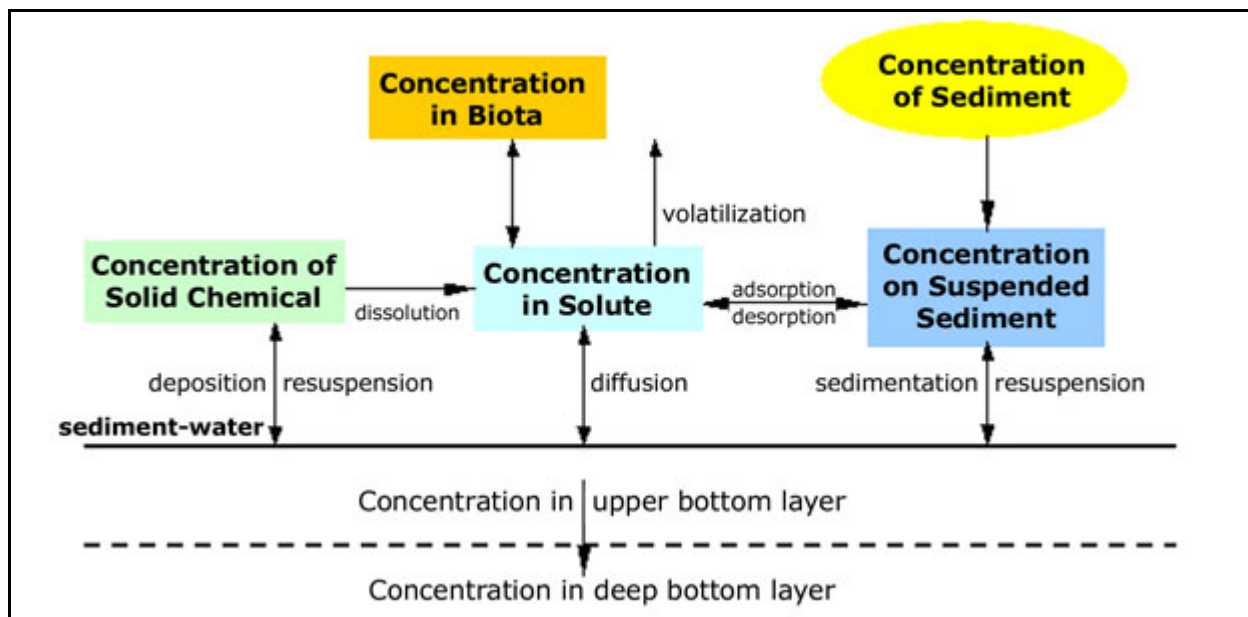


Figure 2. Key process of the chemical transport in stream/channel

The main physical exchange mechanisms are the sedimentation of the contaminated suspended matter into the stream/channel bed and the resuspension of the sediments into water. They are controlled by hydraulic factors (e.g., stream flow, sediment transport), and strongly depend on the sediment size fractionation (e.g., clay, silt, sand and gravel). Chemical diffusion through interstitial water is a process that accounts for migration phenomena not related to sediment transport. Adsorption and desorption of a chemical, dissolution, and decay are the main chemical kinetics processes. Adsorption-desorption from particles occurs with suspended sediments in the water as well as those with the bed sediment.

Chemical transport routing equations. This stream module describes the 1-D advection diffusion transport of the cross-sectionally averaged concentrations of chemicals in the solution, the concentration of chemicals on the suspended sediments, the concentration of solid chemicals, and the concentration in the top layer of the bottom sediment depositions. Adsorption-desorption and diffusive contamination transport in the “water-suspended sediments” system and “water-bottom deposition” system are treated via the distribution coefficient approach, additionally taking into account the exchange rates between water and solid particles for more realistic simulation of the kinetic processes.

Dissolved chemical transport in stream. The 1-D governing mass conservation equation for dissolved (aqueous) chemicals in streams can be written as:

$$\frac{\partial(C_d^r A)}{\partial t} + \frac{\partial(QC_d^r)}{\partial x} = \frac{\partial}{\partial x} \left(D_x A \frac{\partial C_d^r}{\partial x} \right) + \Sigma(C_d^r)_i q_i + \Sigma S \quad (38)$$

where:

C_d^r = dissolved chemical concentration in the stream (M/T³)

D_x = longitudinal dispersion coefficient (L/T²)

λ = chemical first-order decay constant (1/T)

q_l = lateral inflow rate (L²/T)

$(C_d^r)_l$ = dissolved chemical concentration of the surface runoff input to the channel by distributed flows (M/T³)

ΣS = source/sink term, which accounts for changes that are solely biological and chemical (M/ L²/T)

Considering the volatilization, dissolution of particulate phase and chemical exchange between dissolved and adsorbed phases, Equation 38 becomes:

$$\begin{aligned} \frac{\partial(C_d^r A)}{\partial t} + \frac{\partial(Q C_d^r)}{\partial x} = \frac{\partial}{\partial x} \left(D_x A \frac{\partial C_d^r}{\partial x} \right) + \Sigma(C_d^r)_l q_l - \\ \lambda A C_d^r - k_v \frac{A}{H} C_d^r - k_s \frac{A}{H} C_s (k_d^r C_d^r - C_a^r) + k_p \frac{A}{H} (S - C_d^r) \end{aligned} \quad (39)$$

where:

k_v = volatilization rate of the constituent (L/T), the volatilization formulation assumes that chemical concentration in the atmosphere is negligible

H = depth of the stream/channel (L)

k_s = exchange rate between dissolved and adsorbed phases (1/T)

C_a^r = adsorbed chemical concentration on suspended sediments (M/M)

C_s = concentration of the sediment input to the channel by distributed flow (M/T³)

k_p = mass transfer coefficient between the solid and liquid phases (L²/T)

Transport of adsorbed chemical on suspended sediment. The 1-D governing mass transport equation for adsorbed chemicals on suspended sediments in streams can be written as:

$$\begin{aligned} \frac{\partial(C_s C_a^r A)}{\partial t} + \frac{\partial(Q C_s C_a^r)}{\partial x} = \frac{\partial}{\partial x} \left(D_x A \frac{\partial C_s C_a^r}{\partial x} \right) + \Sigma(C_s C_a^r)_l q_l - \\ \lambda A C_s C_a^r + k_s \frac{A}{H} C_s (k_d^r C_d^r - C_a^r) + \frac{A}{H} (q_{res} C_a^s - q_{sed} C_a^r) \end{aligned} \quad (40)$$

where:

- C_a^s = adsorbed chemical concentration in bottom depositions (M/M)
- $(C_a^r)_l$ = adsorbed chemical concentration of the surface runoff input to the channel by distributed flows (M/T³)
- q_{sed} = sedimentation rate (M/L²/T)
- q_{res} = resuspension rate of the bed sediments (M/L²/T)

Sediment resuspension is implied when settling of the sediments is less than settling through the water column.

The parameterization of the sedimentation and resuspension rates is given by the watershed sediment transport module. The sediment transport models are based on the suspended sediment mass conservation equation with the sink-source term describing sedimentation-resuspension rate and the equation of bottom deformation. A physically based approach calculates these rates as a function of the difference between the actual and the equilibrium concentration of the suspended sediments.

Particulate solid chemical transport in streams. Separate particulate chemical transport is described by the following advection-dispersion equations with the sink-source term describing solid chemical deposition-resuspension exchange processes similar with the sediment transport:

$$\begin{aligned} \frac{\partial(C_p^r A)}{\partial t} + \frac{\partial(Q C_p^r)}{\partial x} = \frac{\partial}{\partial x} \left(D_x A \frac{\partial C_p^r}{\partial x} \right) + \Sigma (C_p^r)_l q_l \\ - \lambda A C_p^r - k_p \frac{A}{H} (S - C_d^r) + \frac{A}{H} (q_{res}^p - q_{sed}^p) \end{aligned} \quad (41)$$

where:

- C_p^r = particulate chemical concentration in stream (M/L³)
- $(C_p^r)_l$ = particulate chemical concentration of the surface runoff input to the channel by distributed flows (M/L³)
- q_{sed}^p = solid chemical deposition rate (M/L²/T)
- q_{res}^p = solid chemical resuspension rate of the bed sediments (M/L²/T)

Chemical transfer in bed sediment. Bed sediments are envisioned as a single, well-mixed layer (Figure 2). Chemicals are exchanged with the overlying water through settling of the particulate fraction and diffusion of the dissolved fraction. Within the sediments, chemicals undergo decay and burial to deep, inactive sediments. The sediment-water interface is complex and not always a definite plane that separates solid particles and water. Adsorbed chemical transfer of the bed sediment is described by the following mass conservation equation:

$$\frac{\partial C_a^s \Delta z}{\partial t} = -\lambda C_a^s \Delta z + \frac{1}{\rho_s (1 - \varepsilon)} (q_{sed} C_a^r - q_{res} C_a^s) \quad (42)$$

where:

ε = porosity of the bottom sediments

ρ_s = density of bed sediments (M/T³)

Decay rates and partition coefficients within the sediments may vary from those specified for the water column.

The solid chemical mass conservation equation of the bed sediment can be written as:

$$\frac{\partial C_p^s \Delta z}{\partial t} = -\lambda C_p^s \Delta z + (q_{sed}^p - q_{res}^p) - k_p (S - C_d^r) \quad (43)$$

where C_p^s is particulate chemical concentration in bed sediment (M/L³).

Fluxes of sedimentation and resuspension control the dynamics of the uppermost contaminated layer of the bottom sediments. The thickness of this layer is given by the stream sediment transport module and could be calculated from the sediment mass conservation equation:

$$\rho_s (1 - \varepsilon) \frac{\partial \Delta z}{\partial t} = (q_{sed} - q_{res}) \quad (44)$$

CAMP SHELBY: Camp Shelby, Mississippi, the largest state-owned training site in the nation, has a long history of serving the country, and is considered by many as “a national treasure.” During wartime, the camp's mission is to serve as a major, independent mobilization station of the U.S. Army Forces Command (FORSCOM). The Camp Shelby Training Site is the largest reserve component training site in the United States, covering 136,000 acres, allowing up to battalion level maneuver training, excellent FA firing points, and a wide range of support facilities. This is the normal annual training location for National Guard and Reserve units located in Mississippi, Alabama, and Tennessee. However, units from across the country use its excellent assets to support a variety of missions.

Camp Shelby has been designated as a Power Support Platform (PSP) tasked to mobilize, receive, train, and support Reserve Component (RC) units required to expand the Active Army Component (AC) to meet emergency requirements.

Along with Camp Atterbury, IN, Camp Shelby was one of only two Guard facilities activated, as of late July 2004, as mobilization centers for overseas deployment.

The impact area at Camp Shelby is used for the firing of small- and large-caliber weapons and consists of approximately 17 km² of gently rolling grassland. A number of streams drain the impact area, and riparian wetlands are common along these streams. The impact area is utilized

year-around and averages in excess of 190 firing days each year; there are approximately 170 troop-firings per day, and the range-firing list includes M1A1 tanks, Bradleys, self-propelled and towed artillery, mortars, laser-guided weapons, and small arms.

Like the rest of the Deep South, Camp Shelby has hot, humid summers and relatively mild winters. Winter temperatures run 31 to 60 °F/-1 to 15 °C, though they can drop to 32 °F/0 °C or lower on occasion. Though mild, winter has the most rainfall. High humidity and temperatures of 90 °F/32 °C and higher are common in summer. Spring and fall are mild, with comfortable temperatures and humidities. Expect March-May to provide temperatures from 43 to 85 °F/6 to 29 °C, with humidity running in the 54- to 85-percent range (humidity levels tend to decrease in the midday and afternoon hours).

SITE DATA: Meetings, e-mails, and phone conversations have been held with the Mississippi National Guard, the National Forestry Service, and the University of Southern Mississippi in regard to existing data to support numerical model development at Camp Shelby. From these contacts, the following data have been identified:

- Digital elevation map.
- Soil texture.
- Land use/land cover.
- Meteorological data.
- Stream flow data.
 - o Middle Creek (USGS).
 - o Poplar Creek (possibly).
 - o Pearce Creek (next FY).
- 1200 drilling logs and geophysical logs (Perry and Forest Counties).

Data needs that have been identified are:

- Contaminant source and loading for the impact area.
- Contaminant physical characteristics.
- Critical contaminant parameters (i.e., distribution coefficients for “water-suspended sediment” and “water-upper soil layer” systems, dissolved mass transfer coefficient for “water-upper soil layer” system, dispersion coefficient in overland flow and vadose...etc.).
- Continued flow monitoring.
- Suspended and bedload sediment sampling.
- Dissolved, adsorbed, and particulate contaminant sampling.

Digital elevation data were downloaded from the USGS. The data are at 30-m resolution and cover the watershed area, Figure 3. This data set will be used to determine the flow direction and slope for both the overland and channel grid cells.

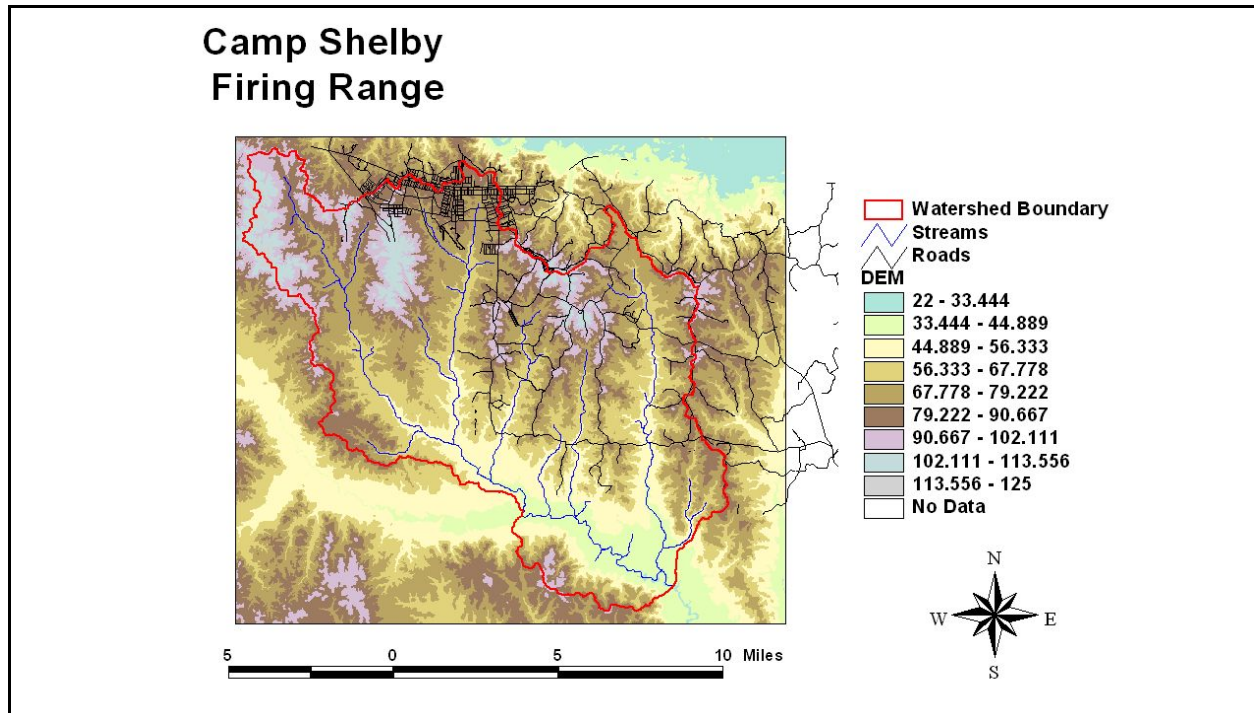


Figure 3. Digital elevation map (meters)

Three sources of soil texture were provided: 1) Mississippi National Guard, Figure 4; 2) SSURGO Database, Figure 5; and 3) STATSGO Database, Figure 6. All of these data cover some extent of the watershed at varying degrees of resolution. These three data sources will be merged to create the most detailed soil texture map of the watershed area.

Attempts were made to find more detailed landuse/land cover data; however, the most detailed and comprehensive dataset was made available by the USGS, Figure 7. All LULC features are delineated by curved or straight lines that depict the actual boundary of an area, commonly referred to as a polygon. These polygons have a minimum size of 10 acres or 4 ha. Each polygon represents a homogeneous element in the mapping scheme that is labeled with an integer or attribute code. The minimum area representing the manmade features of the LULC polygons are 10 acres (4 ha) that have a minimum width of 660 ft (200 m). This minimum width precludes the existence of very narrow or long tracts of data classification. Non-urban and non-manmade features may be mapped with polygons with a minimal area of 40 acres (16 ha) that have a minimum width of 1,320 ft (400 m).

Dr. David Patrick, University of Southern Mississippi, provided a digital copy of the well database created by his team for Camp Shelby, Figure 8. Presently, ERDC is evaluating these well data in an effort to see if they can be used for creating the subsurface features necessary to model contaminants in the groundwater.

The Mississippi National Guard provided a georeferenced aerial photograph, Figure 9. These data can be used to check the land use data provided by the USGS in addition to assisting other team members in creating an estimated contaminant loading map for use in the modeling.

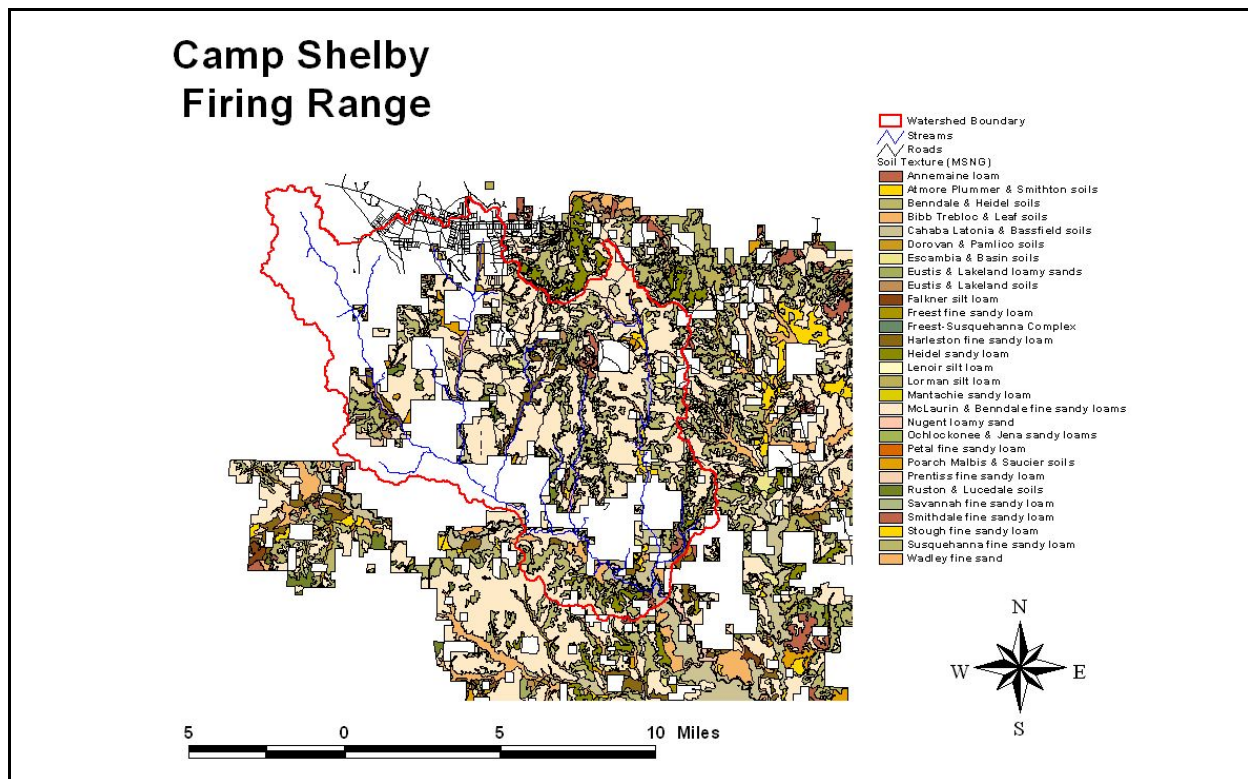


Figure 4. Soil texture map furnished by Mississippi National Guard

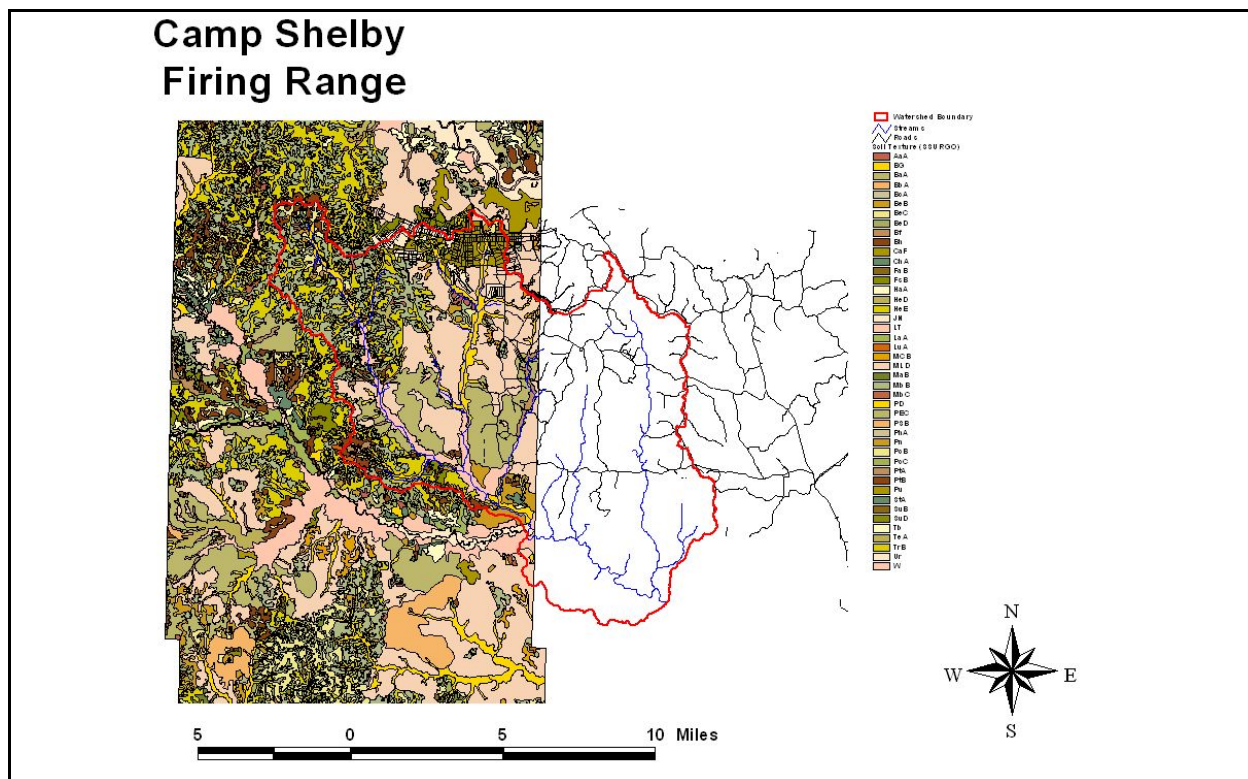


Figure 5. Soil texture map (SSURGO Database)

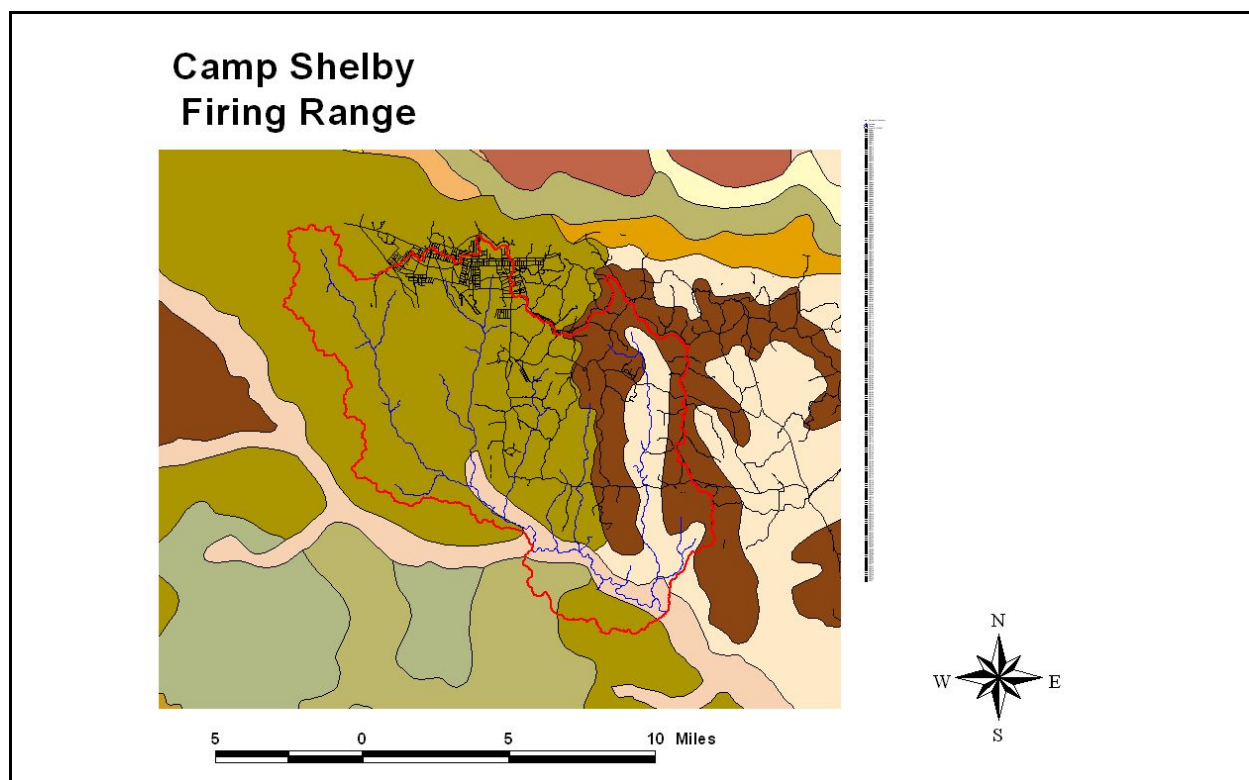


Figure 6. Soil texture map (STATSGO Database)

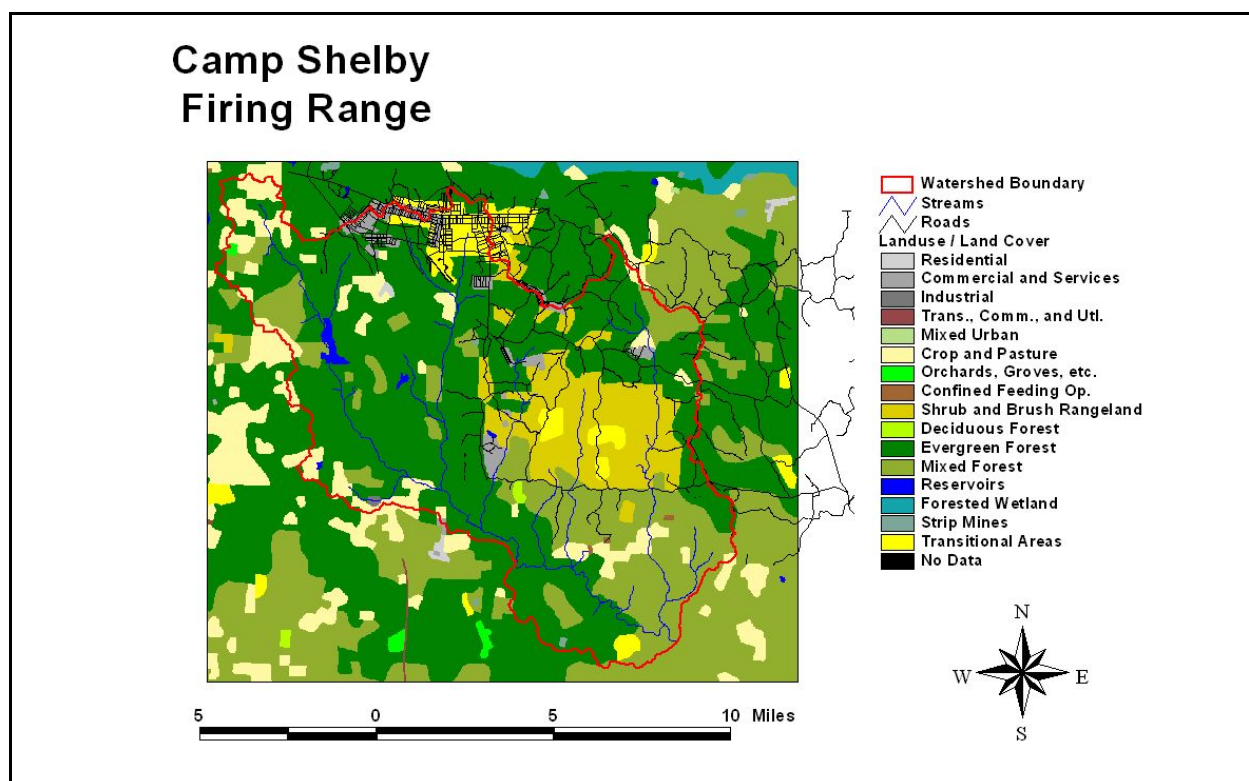


Figure 7. Land use/land cover map (USGS)

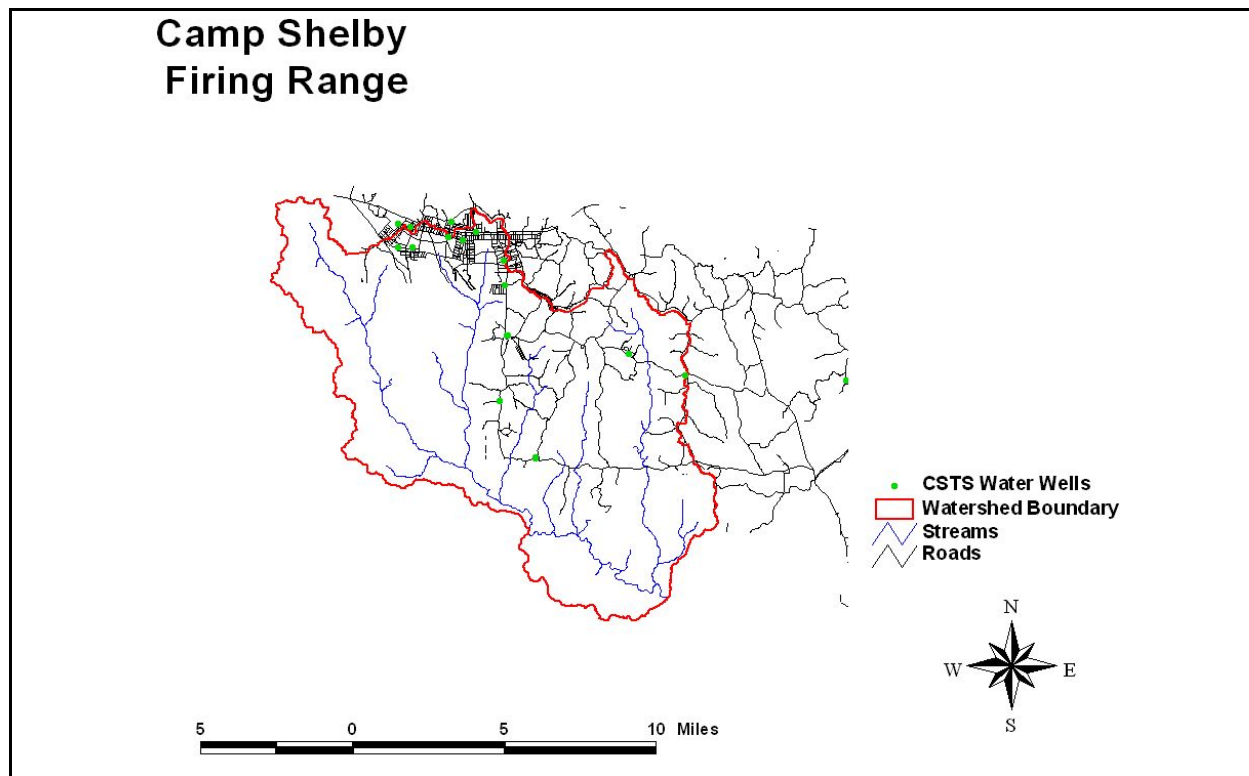


Figure 8. CSTS water well locations

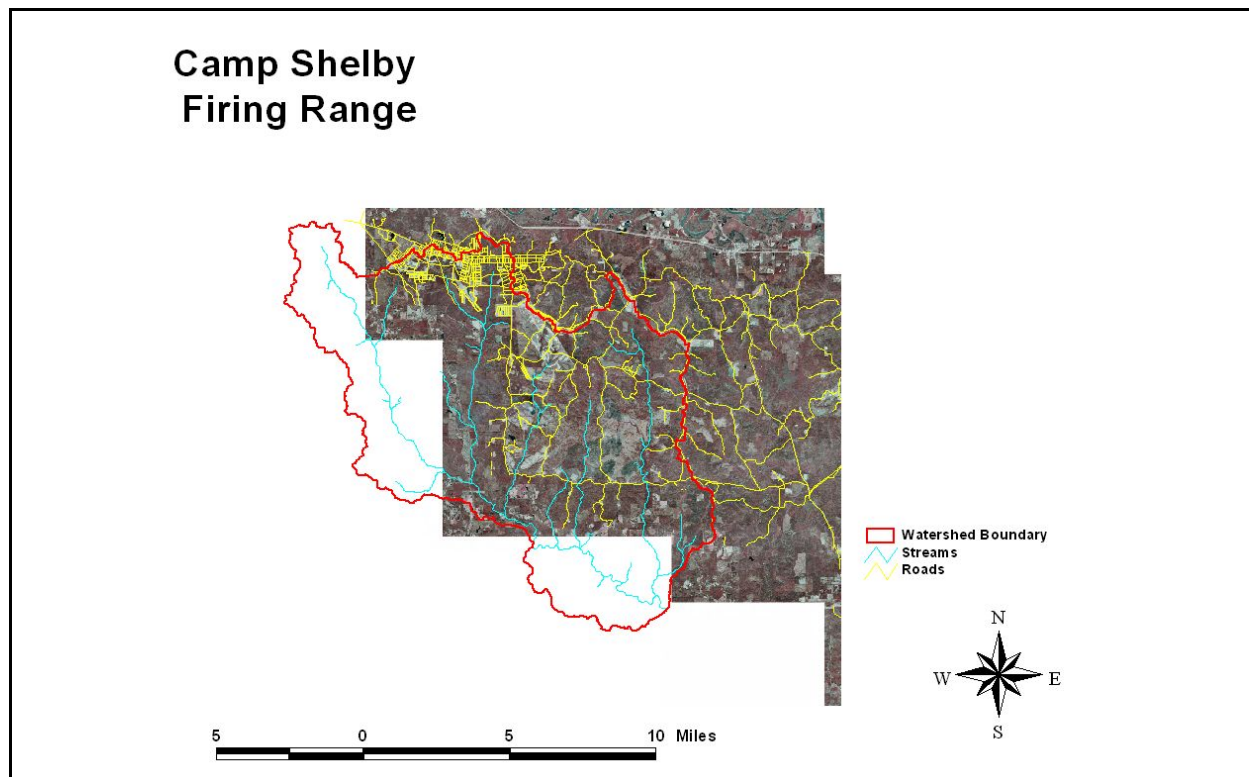


Figure 9. Aerial photography furnished by Mississippi National Guard

Camp Shelby recently set up two weather stations that are collecting the following data: wind speed and direction, precipitation, temperature, and humidity. The periods of record are as follows, Tables 1-3:

Table 1 8/5/2003 to 9/5/2003 Period of Record			
Serial Number	Data Type	Start Date/Time	End Date/Time
594286	Series: Wind speed (m/s) #521003-1	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Wind speed (MPH) #521003-1	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Gust speed (MPH) #521003-2	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Rain (mm) #536472	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Rain (in) #536472	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Temperature (*F) #549371-1	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Dew point (*F) #549371-1	8/5/2003 10:55	9/5/2003 9:35
594286	Series: RH (%) #549371-2	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Pressure (mbar) #595717	8/5/2003 10:55	9/5/2003 9:35
594286	Series: Pressure (in Hg) #595717	8/5/2003 10:55	9/5/2003 9:35

Table 2 8/7/2003 to 6/2/2004 Period of Record			
Serial Number	Data Type	Start Date/Time	End Date/Time
599209	Series: Rain (mm) #533321	8/7/2003 10:35	6/2/2004 13:35
599209	Series: Rain (in) #533321	8/7/2003 10:35	6/2/2004 13:35
599209	Series: Pressure (mbar) #595713	8/7/2003 10:35	1/12/2004 9:35
599209	Series: Pressure (in Hg) #595713	8/7/2003 10:35	1/12/2004 9:35
599209	Series: Temperature (*F) #599831-1	8/7/2003 10:35	6/2/2004 13:35
599209	Series: Dew point (*F) #599831-1	8/7/2003 10:35	6/2/2004 13:35
599209	Series: RH (%) #599831-2	8/7/2003 10:35	6/2/2004 13:35

Table 3 1/22/2004 to 6/2/2004 Period of Record			
Serial Number	Data Type	Start Date/Time	End Date/Time
594286	Series: Wind speed (m/s) #521003-1	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Wind speed (MPH) #521003-1	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Gust speed (MPH) #521003-2	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Rain (mm) #536472	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Rain (in) #536472	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Temperature (*F) #549371-1	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Dew point (*F) #549371-1	1/22/2004 12:40	6/2/2004 12:00
594286	Series: RH (%) #549371-2	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Pressure (mbar) #595713	1/22/2004 12:40	6/2/2004 12:00
594286	Series: Pressure (in Hg) #595713	1/22/2004 12:40	6/2/2004 12:00

On July 15, 2004, the USGS, in cooperation with ERDC, set up and started collecting stream stage and stream flow data at Middle Creek, Figures 10 and 11. These data are being collected every 5 minutes and can be downloaded via the web.

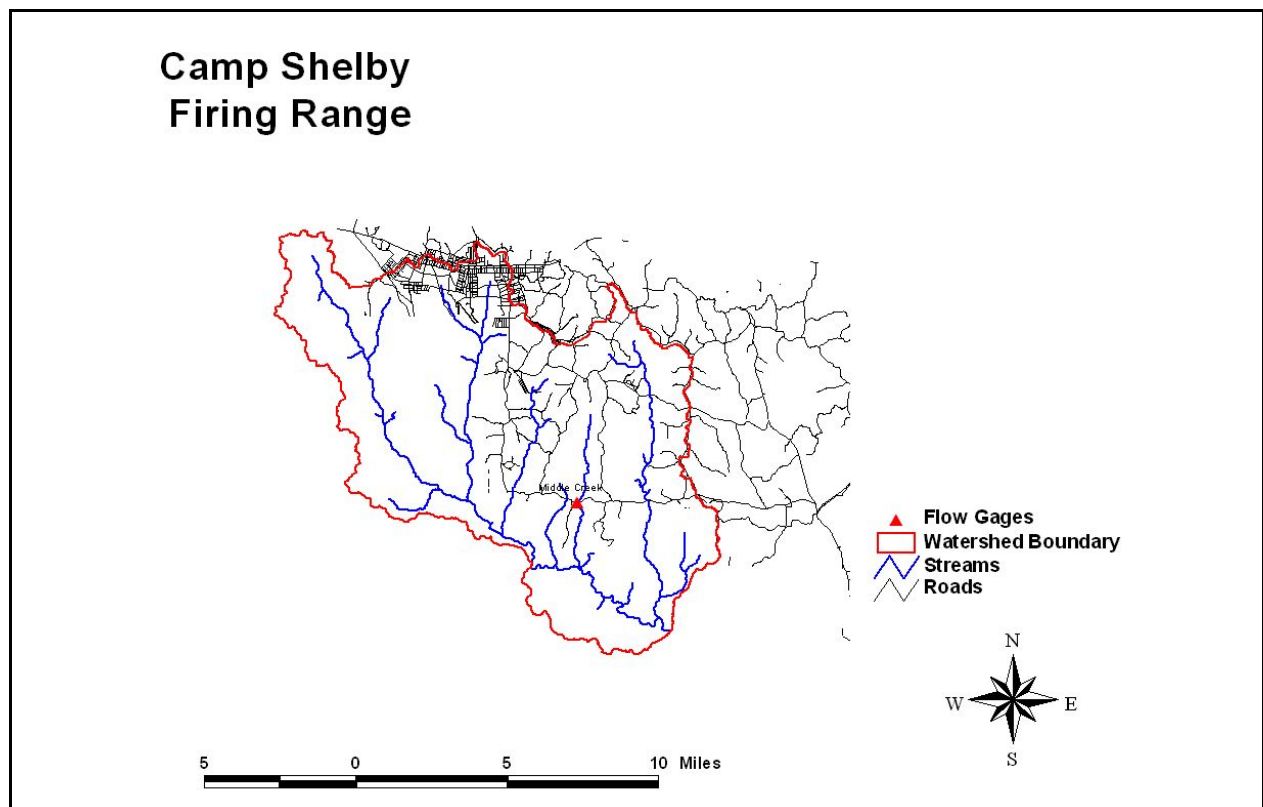


Figure 10. USGS flow gauge at Middle Creek

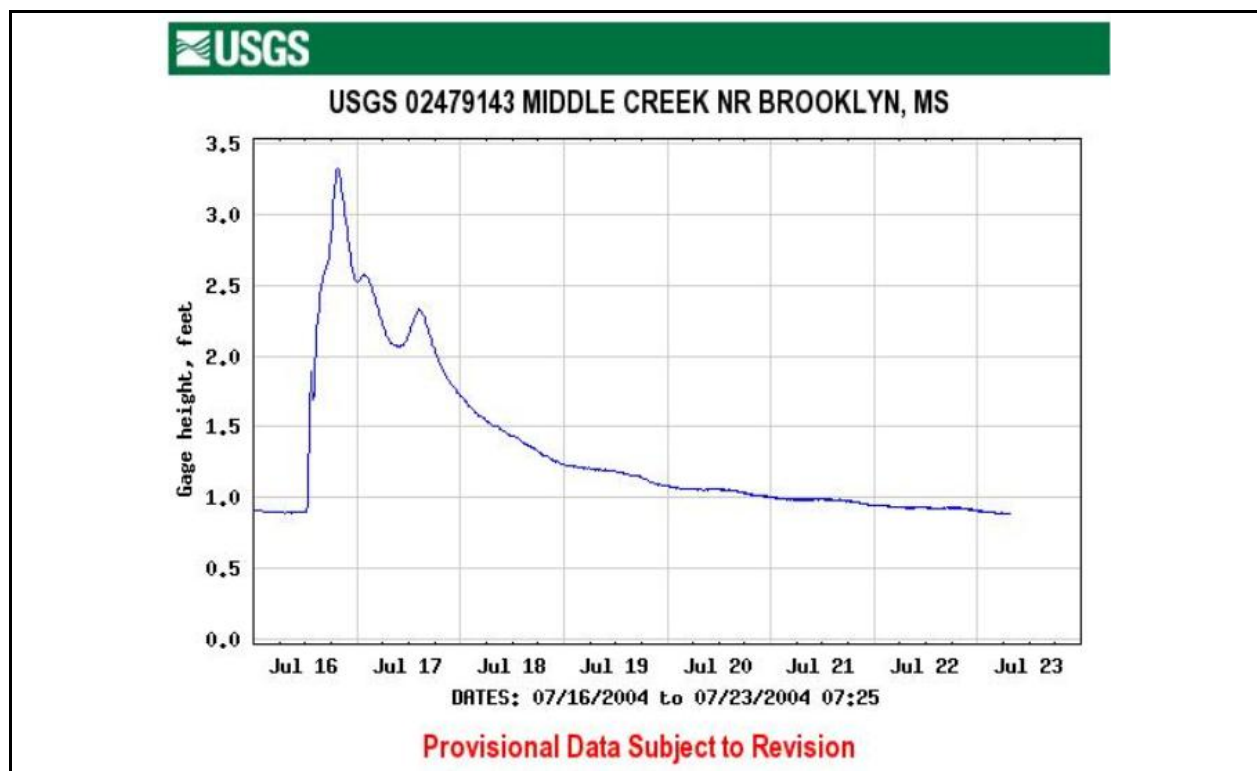


Figure 11. Sample gauge output data (stage) at Middle Creek

In FY05, ERDC will again be working with the USGS to install and monitor a stream stage and stream flow gauge on Pearce Creek. Presently, a gauge site has not been decided upon; however, a site map, Figure 12, showing the major streams for the watershed. These gage data will be collected every 5 minutes and will be downloaded via the web. In addition to collection flows, ERDC will investigate the possibility of collecting sediment and contaminant samples at these gauging locations. Collection of these data sets will allow ERDC scientists and engineers to test their understandings of the fate and transport of military contaminants in addition to calibrating and verifying the distributed source model for Camp Shelby.

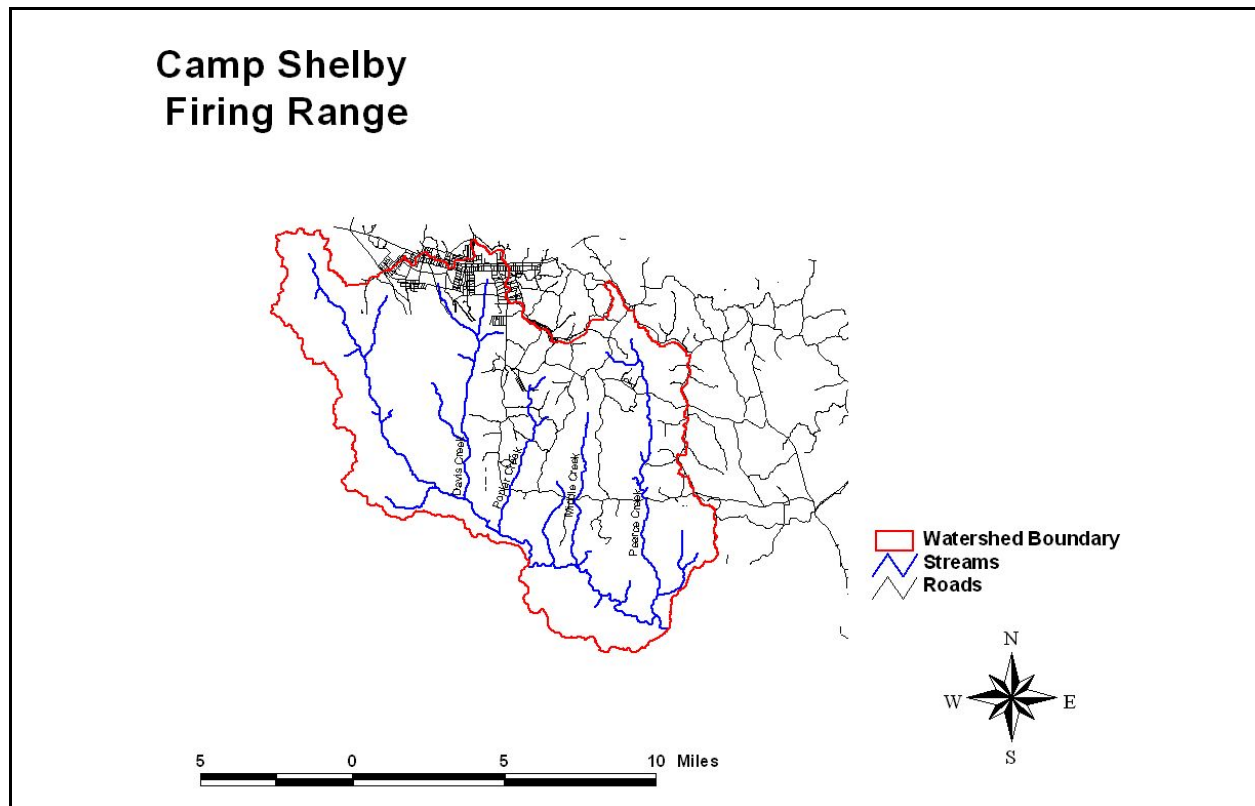


Figure 12. Major tributaries

Future Data Needs. The following items have been identified as data needs to complete the Camp Shelby watershed model and to calibrate and verify the contaminants being transported through the system.

- Channel cross sections. WQCMB will do a field reconnaissance to gather channel geometry. Bottom widths, top widths, and side slopes will be measured and Manning's 'n' estimations will be made from field observations.
- Mass loading map for military contaminants (Comp. B and C4). For TNT and RDX for each explosive, an initial mass loading map will be developed for the model. ERDC scientists have estimated that Comp. B is composed of 60 percent RDX and 39 percent TNT while C4 is composed of 90 percent RDX and 10 percent TNT. Impact areas (craters), mass at the center, and distribution of mass as one moves from the center of the crater need to be estimated. Once this is done, then a GIS analysis can be done to develop an initial mass

loading map for Comp. B and C4. By knowing the percentages of RDX and TNT for each explosive, an initial RDX and an initial TNT mass loading map can be computed.

- At each flow gauge site, water samples and bed samples will be collected. The water samples need to be evaluated for sediment gradation, dissolved contaminants, particulate contaminant, and contaminants adsorbed to any suspended sediment (i.e., silt and clay particles). The bedload samples need to be evaluated for sediment gradation, contaminant particulate, and contaminants adsorbed to bedload sediments.
- One flow gauge located at Middle Creek currently measures stages and computes flowings via a USGS discharge rating curve. The same observed data sets need to be measured at Pearce Creek.
- Meteorological station is currently being maintained at Camp Shelby. These data appear to be sufficient for this development effort. Further data investigations will be pursued to enhance the meteorological coverage of the area.
- Soil borings and groundwater levels have been received from the University of Southern Mississippi. These soil borings and water levels should be sufficient to develop the groundwater flow components of the model. As more subsurface information becomes available, it will be incorporated into the model.
- Digital elevation maps (30 m) have been downloaded and used to create the watershed boundary, watershed topology, and stream network. These data are deemed to be sufficient for this study. If LIDAR information becomes available, then the elevation grid may be updated to reflect more accurate topology.
- Land-use maps have been downloaded from the USGS. Given the relatively sparse nature of the watershed, these maps should be sufficient. As aerial photography or more detailed land-use maps become available, they will be incorporated into the modeling system.
- Soil texture maps have been downloaded from the USDA. For some regions of the watershed, the soil texture is sufficient; however, detailed soil texture was not available for the eastern portion of the watershed, so the STATSGO database was used. As more detailed soil texture data become available for the eastern portion of the watershed, those data will be incorporated into the model.
- Partitioning coefficients between particulate, dissolved, and adsorbed contaminant phases are needed for all contaminants.
- Child products and transfer rates between parent material (i.e., TNT and RDX), and child products are needed.

POINT OF CONTACT: For additional information, contact Billy Johnson (601-634-3425, Billy.E.Johnson@erdc.usace.army.mil). This technical note was written by Mr. Johnson, U.S. Army Engineer Research and Development Center, Environmental Laboratory, and Mr. Zhonglong Zhang, ASI, Inc. This technical note should be cited as follows:

Johnson, B. E., and Zhang, Z. (2005) "Development of a distributed source contaminant transport model for ARAMS," *SERDP Technical Notes Collection* (ERDC/EL TN-ECMI-05-3), U. S. Army Engineer Research and Development Center, Vicksburg, MS. <http://el.erdc.usace.army.mil>

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