ERDC/EL TR-07-XX

Environmental Laboratory

US Army Corps
of Engineers®
Engineer Research and
Development Center

System Wide Water Resources Program - Nutrient Sub-Model (SWWRP-NSM) version 1.1

Billy Johnson, Terry Gerald, and Zhonglong Zhang

March 2007

Approved for public release; distribution is unlimited.

System-Wide Water Resources Program

ERDC/EL TR-07-XX
March 2007

System Wide Water Resources Program - Nutrient Sub-Model (SWWRP-NSM) version 1.1

Billy Johnson, Terry Gerald and Zhonglong Zhang

Environmental Laboratory
U.S. Army Engineer Research and Development Center
3909 Halls Ferry Road
Vicksburg, MS 39180

Draft report

Prepared for U.S. Army Corps of Engineers
Washington, DC 20314-1000

Contents

Figures

Preface

This report summarizes the development efforts undertaken in developing a nutrient sub-model for linkage with a variety of hydraulic and hydrologic modeling systems since the release of SWWRP-NSM version 1.0. This development effort was performed by the Engineer Research and Development Center (ERDC), Waterways Experiment Station, Vicksburg, Mississippi. Funding was provided under the System Wide Water Resources Program (SWWRP). Appreciation is extended to all those who assisted in the formulations and review of the process descriptions implemented within the Nutrient Sub-Model (NSM).

Principal Investigators for this study were Dr. Billy E. Johnson of the Water Quality and Contaminant Modeling Branch (WQCMB), Dr. Zhonglong Zhang of SpecPro Inc., and Mr. Terry K. Gerald of SpecPro Inc. Dr. Zhang and Mr. Gerald were funded as onsite contractors under Task Order Contract W912HZ-05-D-0011 on Civil Delivery Order No. 15. Dr. Johnson conducted his portion of the study under the general supervision of Dr. Barry W. Bunch, Chief of WQCMB, and under the general supervision of Dr. Richard E. Price, Chief of EPED, and Dr. Beth C. Fleming, Director of EL.

COL. Richard B. Jenkins, EN, was Commander and Executive Director of ERDC. Dr. James R. Houston was Director.

This report should be cited as follows:

Johnson, B.E., Gerald, T.K. and Zhang, Z. (2007). "System Wide Water Resources Program - Nutrient Sub-Model (SWWRP-NSM) version 1.1" ERDC/EL TR-07-X, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

1 Introduction

Non-point source (NPS) runoff of pollutants is viewed as one of the most important factors causing impaired water quality in freshwater and estuarine ecosystems and has been addressed as a national priority since the passage of the Clean Water Act, Section 319 (33USC $1329). Nutrients are conveyed to water bodies from watershed, atmospheric and oceanic sources. To assist with compliance of water quality regulations as well as long-term watershed planning and management, there is a need in developing advanced watershed water quality models.

Within the System Wide Water Resources Program (SWWRP), multiple riverine, estuarine, watershed, and subsurface flow models are being modified to address issues of environmental concern. Several integration approaches are either ongoing or proposed to accomplish this task. To have a full system-wide water quality and contaminant capability in SWWRP, the different hydrologic and hydraulic engines must utilize a common water quality and contaminant approach to prevent the arbitrary partitioning of state variables. The goal of this development effort is to upgrade existing hydrologic and hydraulic models (i.e., water engines) using a common water quality approach in order to facilitate their linkage and application on a system wide basis.

In keeping with a common water quality approach to model development, a library of water quality kinetic modules are being developed such that they can be integrated with a variety of water transport engines. The library of algorithms has the following characteristics:

- Multi-species, multi-phase, and multi-reaction system
- Fast (equilibrium-based) and slow (non-equilibrium-based or rate-based) reactions
- Easily extensible to new reaction pathways
- Includes both common nutrient and contaminant packages as well as geochemistry
- Simple, well-defined data interface and calling procedure

The water quality modules are developed such that they are data structure independent thus facilitating their integration into a wide range of modeling systems.

The Nutrient Sub-Model (NSM) has been developed as a library of water quality kinetic modules. NSM considers detailed Nitrogen (N) and Phosphorus (P) cycling and computes nutrient kinetic fluxes for nitrogen and phosphorus at the watershed scale. Modeling of nutrients within NSM consists of three distinct parts:

- Simulating the N and P cycle in the soil
- Transformation and loading of N and P species in the overland flow
- Simulation of the N and P cycle in the water column (both overland and channel)

NSM is written in a modular/process structure facilitating the coupling with hydrologic and hydrodynamic (H&H) model (e.g. HEC-RAS, ADH, HEC-HMS, GSSHA) transport components. Concentrations for each nutrient species are simulated spatially, and are updated at each computational time step, along with water flow and solute transport.

This report describes partitioning of N and P between the dissolved state and the adsorbed state in overland and stream flow, the mass transfer of nutrients between the soil layer (or river/lake bed layer) and the overlying water column, the erosion and sedimentation of nutrients, and the current soil plant dynamics available within NSM. Nutrient kinetic process theory and formulations for overland and channel flow are described in detail in Johnson and Gerald, (2006) and will not be discussed in this report.

2 Partitioning of Nutrients in Surface Runoff

Nitrogen

Soil nitrogen occurs in several chemical forms, which vary greatly not only in their characteristics but also in behavior. Soil nitrogen forms are classified as either organic or inorganic nitrogen. Typically, most nitrogen in soils and surficial sediments occurs in organic form. Organic forms of nitrogen are found in compounds such as amino acids, protein, and more resistant nitrogen compounds (ultimately, humus). Organic nitrogen pools are differentiated on the basis of their carbon to nitrogen ratio (C:N). Organic nitrogen and NH_4^+ are mostly absorbed by clays and can be moved with the soil during erosion. In such forms, nitrogen can be considered immobile. Inorganic forms include ammonium (NH_4^+), nitrate (NO_3^-), and lower concentrations of nitrite (NO_2^-). More importantly, however, NH_4^+ and NO_3^- are soluble and are mobilized through the soil profile during periods of rain by the process of leaching.

The dominant nitrogen species in waters are dissolved inorganic nitrogen - NH_4^+ , NO_2^- , NO_3^- , dissolved organic nitrogen, particulate organic nitrogen and particulate inorganic nitrogen (Burt et al. 1993). The following nitrogen state variables within the water column are simulated by NSM:

- Particulate Organic Nitrogen
- Particulate Ammonium Nitrogen
- Ammonium Nitrogen (NH_4^+)
- Nitrate Nitrogen (NO_3^-)

Phosphorus

Soil phosphorus can exist in a variety of forms: organic phosphorus bound with carbon and oxygen in plant matter, inorganic phosphorus, and as dissolved (soluble) phosphorus. The major types of organic phosphorus compounds are added to the soil by recycling plant, animal, and microbial remains in the soil environment. Inorganic phosphorus occurs as primary minerals (those derived directly from weathered parent material) and secondary minerals (those formed by precipitation of phosphorus with Al, Ca, and Fe). Organic phosphorus and inorganic phosphorus are associated with the particulate phase. In studies of phosphorus movement from agricultural lands the majority is sorbed onto clay materials and transported as erosion products. Soluble phosphorus exists largely as orthophosphate ions and can vary from 0.01 to 3.0 mg/L with organic phosphorus compounds also present in solution. Phosphorus is generally much less mobile than nitrogen, being strongly adsorbed to soil and organic matter. Consequently, in aquatic studies, the focus is often on the sediment-associated forms of phosphorus as these tend to dominate the total phosphorus flux.

Phosphorus enters surface water primarily as particulate matter and secondarily as dissolved inorganic phosphorus also known as “ortho-P” (H_3PO_4 and its conjugate base forms). The following P state variables within the water column are simulated by NSM:

- Particulate Organic Phosphorus
- Particulate Inorganic Phosphorus
- Dissolved Inorganic Phosphorus

Partitioning of Inorganic Nitrogen and Phosphorus

The physical processes of surface runoff cause pollutants or natural materials to be transported and mixed, or exchanged, with other media. There are primarily two kinds of physical processes by which pollutants are transported in fluids: bulk movement of fluids from one location to another (advection), and random mixing processes (diffusion) within the fluids. This random diffusive process is often termed Fickian transport (Fischer et al., 1979). Besides dissolved species, pollutants that are absorbed on the surfaces of particles or absorbed into particles can also be affected by these hydrologic processes. The mechanisms responsible for sorption include ion exchange, cation bridging, charge transfer, H^+ bonding and van der Waals interactions (Kookana et al. 1998).

In NSM, physical transport of inorganic nutrients (N and P) in surface runoff is subdivided into dissolved nutrients and sediment associated nutrients. Thus, there are two unknown concentrations for each species in surface runoff; the two unknowns require two equations, a mass balance equation for the water column and for the soil layer. For suspended solids, a mass balance equation for the water column is required.

Mathematically the total concentration of a species in the water column, C [M/L^3], is separated into two components:

$$C = C_d + C_p \tag{2.1}$$

where C_d is dissolved concentration of a species [M/L^3] and C_p is particulate concentration of a species [M/L^3].

Given the total concentration and the two phase fractions, the dissolved and particulate concentrations in the water column can be determined as follows:

$$C_d = f_d C \tag{2.2a}$$

$$C_p = \sum_{n=1}^{N} C_p^n = \sum_{n=1}^{N} f_p^n C \tag{2.2b}$$

where f_d, f_p^n are fraction of the total concentration that are in dissolved form and particulate form associated with particle "*n*", respectively. The sum of the two fractions (C_d *and* C_p) is equal to 1, and C_p^n is the particulate concentration of a species associated with particle "*n*" [M/L^3].

The fraction dissolved and fraction particulate in the water column are derived using the distribution coefficients for reversible, linear, equilibrium partitioning between dissolved and sorbed phases and are shown in equations (2.3a) and (2.3b) below:

$$f_d = \frac{1}{1 + \sum_{n=1}^{N} K_d C_s^n} \tag{2.3a}$$

$$f_p^n = \frac{K_d C_s^n}{1 + \sum_{n=1}^{N} K_d C_s^n} \tag{2.3b}$$

With K_d [L^3/M] being the mass transfer coefficient. C_s^n is concentration of suspended particle "*n*" in surface water [M/L^3]; φ is porosity of the upper soil (bed sediment) layer; and ρ_s is dry soil (sediment) density [M/L^3].

For the soils or bed sediments, the fractions associated with dissolved and particulate, respectively, are derived by using porosity:

$$f_{d2} = \frac{1}{\phi + K_{d2}(1-\phi)\rho_s} \tag{2.4a}$$

$$f_{p2} = \frac{K_{d2}(1-\phi)\rho_s}{\phi + K_{d2}(1-\phi)\rho_s} \tag{2.4b}$$

where f_{d2} is fraction of the constituent dissolved in the soil layer (sediment bed); f_{p2} is fraction of the constituent in particulate form in the soil layer (sediment bed); K_d, K_{d2} are mass distribution coefficients for the constituent in the water column and soil layer, respectively [L^3/M].

3 Mass Transfer of Dissolved Nutrients

Mass Transfer Flux

Within the soil or sediment domain, diffusion processes may dominate, while at the soil or sediment surface advection processes are expected to be the dominant processes. The complicated nature of the flux at an interface such as this is usually characterized through the use of a mass transfer coefficient, an empirical coefficient that relates the concentration gradient to mass transport (Choy and Reible 1999).

The transfer rate of dissolved species from the soil to the water column is affected by the concentration gradient across the water-soil interface as well as flow conditions in the water column. Mass transfer theory states that the mass flux of a given species under a given set of flow conditions can be expressed as:

$$S_d = k_e\left(C_{d2}/\phi - C_d\right) \tag{3.1}$$

where S_d is mass transfer flux of a dissolved species [$ML^{-2}T^{-1}$], C_{d2} is dissolved concentration of a species in the soil layer [M/L^3], k_e is mass transfer coefficient between water column and sediment depositions [L/T].

The dissolved concentration in the deposits is described in terms of mass of the substance per bulk volume of the soil layer. In order to get the concentrations of water quality variables in the pore water, the concentrations of the substance of the soil layer must be divided by the porosity as indicated in equation (3.1).

Mass Transfer Coefficient

Overland Flow

Surface-applied or soil incorporated chemicals are often transferred in significant quantities from the soil to surface runoff as a result of rainfall-runoff processes. Several dynamic, inter-related processes control chemical transport from the soil to runoff during rainfall, including ejection of soil water by raindrop impacts, diffusion of chemicals from pore water, infiltration, and soil water-runoff mixing (Zhang et al. 1997; Gao et al. 2004). From early experiments and calculations it has been concluded that only a certain thin soil layer interacts with the rainfall and overland flow. Effective soil depth of interaction is related to the degree of soil aggregation and it increases with land slope, kinetic energy of raindrops, and rainfall intensity

(Ahuja and Lehman 1983; Snyder and Woolhiser 1985).

Gao et al. (2004) developed a model that combined the chemical transfer associated with the raindrop impacts and diffusion by assuming raindrop and diffusion processes could be coupled by superposition. This model captured soil-runoff chemical transfer behavior more realistically than either mixing-layer models or diffusion-based models. From this model, the effective mass transfer coefficient can be expressed as:

$$k_e = k_m + \frac{ai\theta}{\rho_b} \tag{3.2}$$

where a is soil detachability [M/L^3], i is rainfall intensity rate [L/T], θ is volumetric water content, $\rho_b = (1-\phi)\rho_s$ is soil bulk density [M/L^3], k_m is diffusive mass transfer coefficient [L/T], which was derived by the concentration gradient across the hydrodynamic boundary layer (Wallach et al., 1988; Wallach et al., 1989).

Channel Flow

Bed release is an important source of chemical diffuses from bed sediment to the water column. The mass transfer across the sediment-water interface is actually a diffusive flow that is dependent upon the concentration gradient of the dissolved mass between the water column and the benthic sediment. The mass transfer coefficient above bed sediments was summarized as follows by Choy and Reible (1999):

$$k_e = 0.664\,\mathrm{Re}^{0.5}\, S_c^{1/3} \frac{D_e}{L_x}, \qquad \text{for laminar flow boundary layer} \tag{3.3a}$$

$$k_e = 0.036\,\mathrm{Re}^{0.8}\, S_c^{1/3} \frac{D_e}{L_x}, \qquad \text{for turbulent flow boundary layer} \tag{3.3b}$$

where D_e is effective diffusion coefficient [L^2/T], L_x is characteristic length across the sediment-water interface [L], R_e is Reynold number, and S_c is Schmidt number.

4 Erosion and Sedimentation of Particulate Nutrients

The erosion and sedimentation of sediments and associated pollutants shown schematically in Figure 1 are two important processes in water quality modeling. Knowledge of erosion and sedimentation is essential to understanding the transport of pollutants in surface waters. Sediment detachment by surface runoff is usually simulated in terms of a generalized erosion-deposition theory proposed by Smith et al. (1995). This assumes that the transport capacity concentration of the runoff reflects a balance between the two continuous counteracting processes of erosion and deposition. Some of these processes are beyond the scope of this discussion therefore emphasis will be placed on erosion and sedimentation as it relates to nutrients (N and P). In general, the insoluble forms of nitrogen and phosphorus far exceed their soluble forms, the physical transport rate of both inorganic and organic forms of nitrogen and phosphorus with sediment is described as follows.

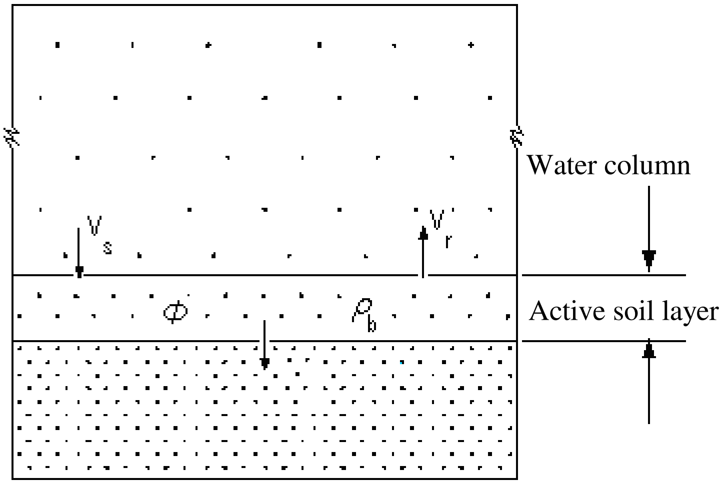

Figure 1. Soil layer (sediment bed) and water interactions for solids

Erosion

Soil erosion involves detachment, transport, and subsequent deposition. Sediment, defined here as eroded soil, is transported down gradient primarily by flowing water. Absorbed on the surface of the sediment particles are chemicals, nutrients, pesticides, and heavy metals. These constituents are eventually deposited into nearby streams and rivers with the entire process being referred to as sedimentation. The products of erosion may be deposited immediately below their sources, or may be transported considerable distances to be deposited in channels, floodplains, or other water bodies. In general, the coarser sediments settle first and the finer particles move further. As a consequence, suspended sediments tend to contain more fines and less dense particles. Because these fine particles usually contain higher amounts of adsorbed chemicals it follows that an enrichment of any sorbed chemical in eroded sediment must be considered and included in water quality modeling. Erosion of the land surface is the major source of solid phase pollutants in surface waters. Within a watershed, the erosion component is divided into upland (hillslope) erosion and channel erosion.

Upland Erosion

Soil erosion may be considered a natural geomorphic process. In performing an analysis, there are a number of erosion mechanisms that need to be taken into account. There are types of erosion in which flowing water and water as raindrops are directly involved in the detachment and movement of sediments as well as a broad class of erosion in which water plays only an indirect role of weakening the soil matrix.

A common description of the soil erosion process involves detachment of soil particles by raindrop impact, transport of this material to rills by sheet flow, and further detachment and transport of soil particles by the rill flow (e.g. Foster et al. 1977). The transport of sediment by overland flow is self-regulating, i.e. soil particle detachment by overland flow does not occur unless there is excess energy available in addition to the amount required to transport suspended sediments. However, detachment by rainfall impact often occurs when there is little or no flow available for transport. Major factors which affect raindrop detachment are the rainfall characteristics, soil characteristics, ground and canopy cover and surface water depth (Taskinen and Bruen 2007).

Channel Erosion

The removal of soil from the banks or beds of streams results in stream channel erosion. Stream channels erode as water flows over the side of the stream bank or scours below the water surface, especially during severe floods. Quantitative estimates of channel erosion can be obtained by similar methods as adopted for upland erosion. The main differences are that soil detachment by raindrop impact within the channel is neglected and that lateral inflows of sediment from the upland become important. Sediment routing within channels involves, as for overland flow, a comparison of the availability of sediment with the transport capacity of the flow.

Erosion Rate of Particulate Nutrients

Within NSM, the formulations have been structured such that the water engines provide the required flow and sediment fluxes necessary to drive the fate and transport of the nutrients.

The transport of nutrient particulates from the soil surface to the water column via erosion occurs at a rate that is proportional to the rate at which sediment particles are eroded (resuspended).

$$S_r = \sum_{n=1}^{N} f_p^n v_r^n C_{s2}^n \tag{4.1}$$

where S_r is total erosion rate of a nutrient $[ML^{-2}T^{-1}]$, C_{s2}^n is particulate concentration associated with particle "*n*" in the soil layer $[M/L^3]$, and v_r^n can be defined as a erosion velocity associated with particle "*n*" [L/T].

Sediments in Surface Water and Deposition

Sediment Characteristics

Sediments are usually associated with streams, rivers, bays, bayous and beaches. Although it would seem that soil and sediment are the same, they tend to be very different in their physical and chemical make up causing their interaction with contaminates to be different. Sediments are less variable in particle size and often contain more organic matter than soil. In addition, sediments in surface water are contaminated with chemicals that sorb onto fine-grained organic and inorganic soil particles.

Sediment is composed of many materials, including individual primary particles, aggregates, organic materials, and associated chemicals. Particles can be mineral or organic in origin. Mineral particles are derived from geologic materials. The density of many mineral particles ranges between 2 and 3 g/cm^3 and are often approximated as 2.65 g/cm^3. Organic particles are derived from plant materials, dead bacterial or algal cells, and decaying aquatic organisms. Organic particles usually have a density only slightly greater than that of water and contain a high fraction of organic carbon, an excellent sorbent for many pollutants.

The role of sediment in water quality pollution is tied both to the particle size of sediment, and to the amount of particulate organic carbon associated with the sediment. Size, shape, and density affect the settling velocity, which in turn affects sediment transport rates and sediment deposition. For phosphorus and metals, particle size (usually 63 μm (silt + clay) fraction) is of primary importance due to the large surface area of very small particles. Phosphorus and metals tend to be highly attracted to ionic exchange sites that are associated with clay particles and with the iron and manganese coatings that commonly occur on these small particles. Many of the persistent, bioaccumulating and toxic organic contaminants, especially chlorinated compounds including many pesticides, are strongly associated with sediment and especially with the organic carbon that is transported as part of the sediment load in surface water.

Deposition Rate of Particulate Nutrients

The magnitude of the deposition flux of a contaminant is equal to the product of the rate of sediment deposition and the contaminant concentration associated with the settling particles. Settling velocity depends not only on the size, shape, and density of particles, but also on the concentration of the particles provided by the water engines.

The deposition of particulate nutrients from the water column is expressed as:

$$S_s = \sum_{n=1}^{N} f_p^n v_s^n C_s^n \tag{4.2}$$

where S_s is total deposition rate of a nutrient [$ML^{-2}T^{-1}$], C_s^n is particulate concentration associated with particle "*n*" in water column [M/L^3], and v_s^n is settling velocity associated with particle "*n*" [L/T].

5 Soil Plant Dynamics

In order to accurately simulate the removal of water and nutrients from the plant root zone, transpiration, and biomass/yield production, a dynamic soil plant module has been developed for NSM. The soil plant algorithms have been taken from the SWAT/EPIC model (Neitsch et al. 2002). Since its inception EPIC has evolved into a comprehensive agro-ecosystem model capable of simulating the growth of crops in complex rotations and management operations, such as tillage, irrigation, fertilization and liming (Williams et al. 1984). This chapter provides a detailed description of the plant growth processes that can be found within the modules.

Currently NSM can simulate approximately 100 plant species including crops, native grasses, and trees. The process descriptions utilize a single plant growth model to simulate all types of land covers. The algorithms are able to differentiate between annual and perennial plants. Annual plants grow from the planting date to the harvest date or until the accumulated heat units equal the potential heat units for the plant. Perennial plants maintain their root systems throughout the year, becoming dormant in the winter months and resume growth when the average daily air temperature exceeds the minimum, or base, temperature required.

For each increment of time, potential plant growth, i.e. plant growth under ideal growing conditions, is calculated. Ideal growing conditions consist of adequate water and nutrient supply and a favorable climate. Differences in growth between plant species are defined by the parameters contained in the plant growth database (Neitsch et al. 2002).

Plant Growth

Plant growth is modeled by simulating leaf area development, light interception and conversion of intercepted light into biomass assuming a plant species-specific radiation-use efficiency (RUE).

Potential Growth

Biomass production

NSM uses the concept of RUE by which a fraction of daily photosynthetically active radiation (PAR) is intercepted by the plant canopy and converted into plant biomass. Daily gains in plant biomass are affected by air vapor pressure deficits and atmospheric CO_2 concentration (Stockle et al. 1992). Stress indices for water, temperature, N, P and aeration are calculated daily using the value of the most severe stress to reduce potential plant growth and crop yield. Similarly, stress factors for soil strength, temperature, and aluminum toxicity are used to adjust potential root growth (Jones et al. 1991).

The amount of daily solar radiation intercepted by the leaf area of the plant is calculated using the Beer's Law (Chapra 1997):

$$R_{phosyn} = 0.5 R_{day} \left[1 - \exp\left(k_l \cdot LAI\right)\right] \tag{5.1}$$

where R_{phosyn} is the amount of intercepted PAR on a given day (MJ m^{-2}), R_{day} is the incident total solar radiation (MJ m^{-2}), $0.5R_{day}$ is the incident PAR (MJ m^{-2}), k_l is the light extinction coefficient, which is taken as -0.65 for all plants, and LAI is the leaf area index for a given day.

PAR is radiation with a wavelength between 400 and 700 mm (McCree 1972). Direct solar beam radiation contains roughly 45% of PAR while diffuse radiation contains around 60% of PAR (Monteith 1972). The fraction of PAR will vary from day to day with variation in cloud cover.

RUE, the amount of dry biomass produced per unit intercepted solar radiation, is defined in the plant growth database, assumed to be independent of the plant's growth stage. The maximum increase in biomass on a given day that will result from the intercepted PAR is assumed to be a linear function of radiant energy (Monteith 1977):

$$\Delta bio = RUE \cdot R_{phosyn} \tag{5.2}$$

where Δbio is the potential increase in total plant biomass on a given day (kg/ha), and RUE is the RUE of the plant (kg/hg $(MJ/m^2)^{-1}$ or 10^{-1} g/MJ).

The total biomass on a given day, d, is calculated as:

$$bio = \sum_{i=1}^{d} \Delta bio_i \tag{5.3}$$

where bio is the total plant biomass on a given day (kg/ha), and Δbio_i is the increase in total plant biomass on a day, i (kg/ha).

Impact of climate on radiation-use efficiency

RUE is sensitive to variations in atmospheric CO_2 concentrations and equations have been incorporated into the EPIC formulations to modify the default RUE values in the plant database for climate change studies. The relationship used to adjust the RUE for effects of elevated CO_2 is given by Stockle et al. (1992):

$$RUE = \frac{100CO_2}{CO_2 + \exp(r_1 - r_2 CO_2)} \tag{5.4}$$

where CO_2 is the concentration of carbon dioxide in the atmosphere (parts per million by volume, or ppmv), r_1 and r_2 are shape coefficients, r_1 is the first shape coefficient, r_2 is the second shape coefficient.

The shape coefficients are calculated by solving equation 5.4 using two known points (RUE_{amb}, CO_{2amb}) and (RUE_{hi}, CO_{2hi}):

$$r_1 = \ln\left[\frac{CO_{2amb}}{(0.01RUE_{amb})} - CO_{2amb}\right] + r_2 CO_{2amb} \tag{5.5a}$$

$$r_2 = \frac{\left(\ln\left[\frac{CO_{2amb}}{(0.01RUE_{amb})} - CO_{2amb}\right] - \ln\left[\frac{CO_{2hi}}{(0.01RUE_{hi})} - CO_{2hi}\right]\right)}{CO_{2hi} - CO_{2amb}} \tag{5.5b}$$

where CO_{2amb} is the ambient atmospheric CO_2 concentration (ppmv), RUE_{amb} is the RUE of the plant at ambient atmospheric CO_2 concentration (kg/hg $(MJ/m^2)^{-1}$ or 10^{-1} g/MJ), CO_{2hi} is an elevated atmospheric CO_2 concentration (ppmv), RUE_{hi} is the RUE of the plant at the elevated atmospheric CO_2 concentration, CO_{2hi}, (kg/hg $(MJ/m^2)^{-1}$ or 10^{-1} g/MJ).

Equation 5.4 was developed when the ambient atmospheric CO_2 concentration was 330 ppmv and is valid for CO_2 concentrations in the range of 330-660 ppmv. Even though the ambient atmospheric concentration of CO_2 is now higher than 330 ppmv, this value is still used in the calculation. If the CO_2 concentration used in the simulation is less than 330 ppmv, the model defines RUE = RUE_{amb}.

Stockle and Kiniry (1990) have shown that a plant's RUE is affected by air vapor pressure deficit. For a plant, a threshold vapor pressure deficit is defined at which the plant's RUE begins to drop in response to the vapor pressure deficit. The adjusted RUE is calculated:

$$RUE = RUE_{vpd=1} - \Delta rue_{dcl}\left(vpd - vpd_{thr}\right) \quad \text{if vpd > vpd}_{\text{thr}} \tag{5.6a}$$

$$RUE = RUE_{vpd=1} \quad \text{if vpd <= vpd}_{\text{thr}} \tag{5.6b}$$

where $RUE_{vpd=1}$ is the RUE for the plant at a vapor pressure deficit of 1 kPa (kg/hg $(\text{MJ/m}^2)^{-1}$ or 10^{-1} g/MJ), Δrue_{dcl} is the rate of decline in RUE per unit increase in vapor pressure deficit (kg/hg $(\text{MJ/m}^2)^{-1}$ or 10^{-1} g/MJ), vpd is the vapor pressure deficit (kPa), and vpd_{thr} is the threshold vapor pressure deficit above which a plant will exhibit reduced RUE (kPa).

The RUE value reported for the plant in the plant growth database, RUE_{amb}, or adjusted for elevated CO_2 levels (Equation 5.4) is the value used for $\text{RUE}_{\text{vpd=1}}$. The threshold vapor pressure deficit for reduced RUE is assumed to be 1.0 kPa for all plants (vpd_{thr} = 1.0). The RUE is never allowed to fall below 27% of RUE_{amb}. This minimum value was based on field observations (Neitsch et al. 2002).

Canopy cover and height

In the initial period of plant growth, canopy height and leaf area development are controlled by the optimal leaf area development curve:

$$fr_{LAI,mx} = \frac{fr_{PHU}}{fr_{PHU} + \exp\left(l_1 - l_2 \cdot fr_{PHU}\right)} \tag{5.7}$$

where $fr_{LAI,mx}$ is the fraction of the plant's maximum LAI corresponding to a given fraction of potential heat units for the plant, fr_{PHU} is the fraction of potential heat units accumulated for the plant on a given day in the growing season, and l_1 and l_2 are shape coefficients.

The fraction of potential heat units accumulated by a given date is calculated:

$$fr_{PHU} = \frac{\sum_{i=1}^{d} HU_i}{PHU} \tag{5.8}$$

where HU_i is the heat units accumulated on day i (heat units), and PHU is the total potential heat units for the plant (heat units).

The shape coefficients are calculated by solving Equation 5.7 using two known points ($\text{fr}_{\text{LAI,1}}$, $\text{fr}_{\text{PHU,1}}$) and ($\text{fr}_{\text{LAI,2}}$, $\text{fr}_{\text{PHU,2}}$):

$$l_1 = \ln\left[\frac{fr_{PHU,1}}{fr_{LAI,1}} - fr_{PHU,1}\right] + l_2 \cdot fr_{PHU,1} \tag{5.9a}$$

$$l_2 = \frac{\left(\ln\left[\frac{fr_{PHU,1}}{fr_{LAI,1}} - fr_{PHU,1}\right] - \ln\left[\frac{fr_{PHU,2}}{fr_{LAI,2}} - fr_{PHU,2}\right]\right)}{fr_{PHU,2} - fr_{PHU,1}} \tag{5.9b}$$

where $fr_{PHU,1}$ is the fraction of the growing season (i.e., fraction of total potential heat units) corresponding to the 1st point on the optimal leaf area development curve, $fr_{LAI,1}$ is the fraction of the maximum plant LAI (i.e., fraction of LAI_{max}) corresponding to the 1st point on the optimal leaf area development curve, $fr_{PHU,2}$ is the fraction of the growing season corresponding to the 2nd point on the optimal leaf area development curve, and $fr_{LAI,2}$ is the fraction of the maximum plant LAI corresponding to the 2nd point on the optimal leaf area development curve.

The canopy height, on a given day, is calculated:

$$h_c = h_{c,\max}\sqrt{fr_{LAI,\max}} \tag{5.10}$$

where h_c is the canopy height for a given day (m), and $h_{c,max}$ is the plant's maximum canopy height (m).

The amount of canopy cover is expressed as the LAI. The leaf area added on day *i* is calculated:

$$\Delta LAI_i = \left(fr_{LAI,\max}{}^{i} - fr_{LAI,\max}{}^{i-1}\right)LAI_{\max}\left[1-\exp\left(5(LAI_{i-1} - LAI_{\max})\right)\right] \tag{5.11}$$

and the total LAI is calculated:

$$LAI_i = LAI_{i-1} + \Delta LAI_i \tag{5.12}$$

where ΔLAI_i is the leaf area added on day i, LAI_i and LAI_{i-1} are the leaf area indices for day i and i-1 respectively, $fr_{LAI,max}{}^{i}$ and $fr_{LAI,max}{}^{i-1}$ are the fraction of the plant's maximum LAI calculated with Equation 5.7 for day i and i-1, and LAI_{max} is the maximum LAI for the plant.

LAI is defined as the area of green leaf per unit area of land (Watson 1947). Once the maximum leaf area index is reached, LAI will remain constant until leaf senescence begins to exceed leaf growth. In general terms, leaf senescence is a way for a deciduous plant to prepare for winter and recycle some of the valuable and often scarce mineral nutrients, such as nitrogen and phosphorus. Leaf senescence is also a way to get rid of old and photosynthetically less efficient leaves in both deciduous and evergreen plants. Once leaf senescence becomes the dominant growth process, the LAI is calculated:

$$LAI = 16 LAI_{mx} \left(1 - fr_{PHU}\right)^2 \qquad \mathrm{fr}_{\mathrm{PHU}} > \mathrm{fr}_{\mathrm{PHU,sen}} \qquad (5.13)$$

where $fr_{PHU,sen}$ is the fraction of growing season (PHU) at which senescence becomes the dominant growth process.

Root development

The amount of total plant biomass partitioned to the root system is 30-50% in seedlings and decreases to 5-20% in mature plants (Jones 1985). Within NSM, the fraction of total biomass in roots varies from 0.40 at emergence to 0.20 at maturity. The daily root biomass fraction is calculated with the equation:

$$fr_{root} = 0.40 - 0.20 fr_{PHU} \qquad (5.14)$$

where fr_{root} is the fraction of total biomass partitioned to roots on a given day in the growing season.

Calculation of root depth varies according to plant type. NSM assumes perennials and trees have roots down to the maximum rooting depth defined for the soil throughout the growing season:

$$z_{root} = z_{root,\max} \qquad (5.15)$$

where z_{root} is the depth of root development in the soil on a given day (mm), and $z_{root,max}$ is the maximum depth for root development in the soil (mm).

The simulated root depth for annuals varies linearly from 0.0 mm at the beginning of the growing season to the maximum rooting depth at $\mathrm{fr}_{\mathrm{PHU}} = 0.40$ using the equation:

$$z_{root} = 2.5 fr_{PHU} \cdot z_{root,\max} \qquad \text{if } \mathrm{fr}_{\mathrm{PHU}} <= 0.40 \qquad (5.16a)$$

$$z_{root} = z_{root,\max} \qquad \text{if fr} > 0.40 \qquad (5.16b)$$

The maximum rooting depth is defined by comparing the maximum potential rooting depth for the plant from the plant growth database and the maximum potential rooting depth for the soil. The smaller of the two is taken as the maximum rooting depth.

Maturity

Plant maturity is reached when the fraction of potential heat units accumulated, fr_{PHU}, is equal to 1.0. Once maturity is reached, the plant ceases to transpire and take up water and nutrients. Simulated plant biomass remains stable until the plant is harvested or killed, result of a management operation.

Actual Plant Growth

Net growth occurs in plants as a function of mortality, respiration requirements, photosynthesis, and demands by the plant organs. The plant growth factor quantifies the fraction of potential growth achieved:

$$\gamma_{reg} = 1 - \max(wstrs, nstrs, pstrs) \qquad (5.17)$$

where γ_{reg} is the plant growth factor and ranges from 0.0 to 1.0.

The potential biomass predicted is adjusted if one of the four plant stress factors is greater than 0.0:

$$\Delta bio_{act} = \Delta bio \cdot \gamma_{reg} \qquad (5.18)$$

The potential leaf area added is also adjusted for plant stress:

$$\Delta LAI_{act,i} = \Delta LAI_i \cdot \sqrt{\gamma_{reg}} \qquad (5.19)$$

Plant growth constraints

In the previous sections, we discussed potential growth. In reality, plant growth may be constrained due to extreme temperatures, and insufficient water, nitrogen, or phosphorus.

Temperature stress

Temperature stress is a function of the daily average air temperature and the optimal temperature for plant growth as the air temperature diverges from the optimal, the plant will begin to experience stress. The equations used to determine temperature stress are:

$$tstrs = 1.0 \qquad \overline{\mathrm{T}}_{\mathrm{av}} <= \mathrm{T}_{\mathrm{base}} \qquad (5.20a)$$

$$tstrs = 1 - \exp\left[\frac{-0.1054\left(T_{opt} - \overline{T}_{av}\right)^2}{\left(\overline{T}_{av} - T_{base}\right)^2}\right] \qquad \mathrm{T}_{\mathrm{base}} < \overline{\mathrm{T}}_{\mathrm{av}} <= \mathrm{T}_{\mathrm{opt}} \qquad (5.20b)$$

$$tstrs = 1 - \exp\left[\frac{-0.1054\left(T_{opt} - \overline{T}_{av}\right)^2}{\left(2T_{opt} - \overline{T}_{av} - T_{base}\right)^2}\right] \qquad \mathrm{T}_{\mathrm{opt}} < \overline{\mathrm{T}}_{\mathrm{av}} <= 2*\mathrm{T}_{\mathrm{opt}}-\mathrm{T}_{\mathrm{base}} \qquad (5.20c)$$

$$tstrs = 1.0 \qquad \overline{\mathrm{T}}_{\mathrm{av}} > 2*\mathrm{T}_{\mathrm{opt}}-\mathrm{T}_{\mathrm{base}} \qquad (5.20d)$$

where *tstrs* is the temperature stress for a given day expressed as a fraction of optimal plant growth, $\overline{\mathrm{T}}_{\mathrm{av}}$ is the mean air temperature for day (^{o}C), T_{base} is the plant's base or minimum temperature for growth (^{o}C), and T_{opt} is the plant's optimal temperature for growth (^{o}C).

Water stress

Water stress is simulated by comparing actual and potential plant transpiration:

$$wstrs = 1 - \frac{E_{t,act}}{E_t} = 1 - \frac{w_{actualup}}{E_t} \qquad (5.21)$$

where *wstrs* is the water stress, $E_{t,}$is the maximum plant transpiration (mm H_2O), $E_{t,act}$ is the actual amount of transpiration on a given day (mm H_2O), and $w_{actualup}$ is the total plant water uptake for the day (mm H_2O).

Nitrogen stress

Nitrogen stress is calculated only for non-legumes. Legumes do not experience nitrogen stress due to nitrogen fixation.

Nitrogen stress is quantified by comparing actual and optimal plant nitrogen levels. Nitrogen stress varies non-linearly between 0.0 at optimal nitrogen content and 1.0 when the nitrogen content of the plant is 50% or less of the optimal value. Nitrogen stress is computed with the following equation:

$$nstrs = 1 - \frac{\varphi_n}{\varphi_n + \exp\left[3.535 - 0.02597\varphi_n\right]} \tag{5.22}$$

where *nstrs* is the nitrogen stress for a given day, and φ_n is a scaling factor for nitrogen stress.

The scaling factor is calculated:

$$\varphi_n = 200\left(\frac{bio_N}{bio_{N,opt}} - 0.5\right) \tag{5.23}$$

where $bio_{N,opt}$ is the optimal mass of nitrogen stored in plant material for the current growth stage (kg N/ha) and bio_N is the actual mass of nitrogen stored in plant material (kg N/ha).

Phosphorus stress

As with nitrogen, phosphorus stress is quantified by comparing actual and optimal plant phosphorus levels. Phosphorus stress varies non-linearly between 0.0 at optimal phosphorus content and 1.0 when the phosphorus content of the plant is 50% or less of the optimal value. Phosphorus stress is computed with the following equation:

$$pstrs = 1 - \frac{\varphi_p}{\varphi_p + \exp\left[3.535 - 0.02597\varphi_p\right]} \tag{5.24}$$

where *pstrs* is the phosphorus stress for a given day, and φ_p is a scaling factor for phosphorus stress.

The scaling factor is calculated:

$$\varphi_p = 200\left(\frac{bio_P}{bio_{P,opt}} - 0.5\right) \tag{5.25}$$

where $bio_{P,opt}$ is the optimal mass of phosphorus stored in plant material for the current growth stage (kg P/ha) and bio_P is the actual mass of phosphorus stored in plant material (kg P/ha).

Water Uptake by Plants

A simple algorithm is used to simulate multiple layer soil water flow, plant water uptake and plant-water relations for a given soil-plant-atmosphere system. The schematic representation in the soil profile is illustrated in Figure 2.

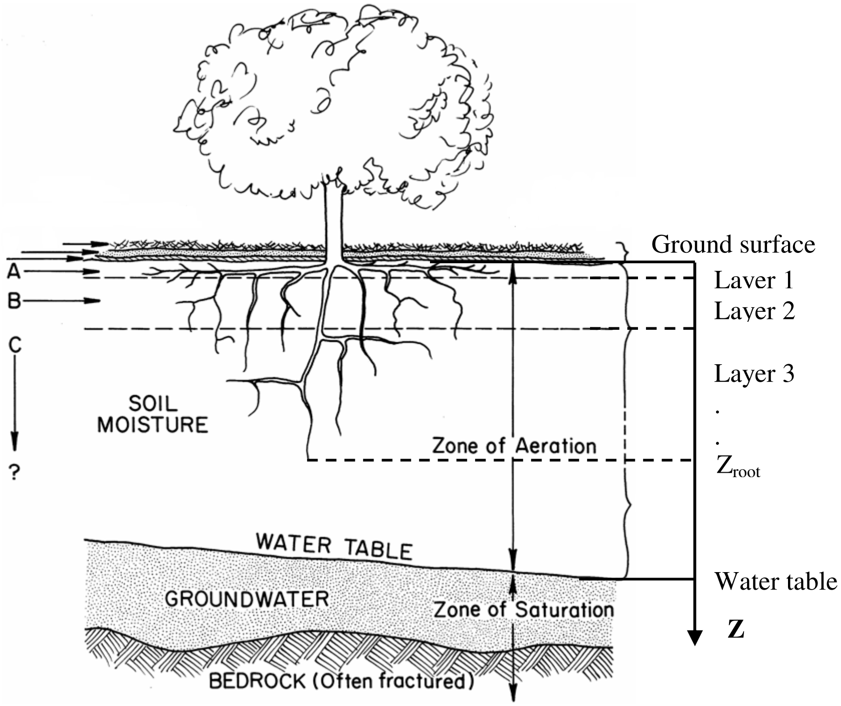

Figure 2. Soil plant dynamics module

The potential water uptake from the soil surface to any depth in the root zone is estimated with the equation:

$$w_{up,z} = \frac{E_t}{\left[1 - \exp(-\beta_w)\right]} \left[1 - \exp\left(-\beta_w \frac{z}{z_{root}}\right)\right] \qquad (5.26)$$

where $w_{up,z}$ is the potential water uptake from the soil surface to a specified depth, z, on a given day (mm H_2O), β_w is the water-use distribution parameter, and z is the depth from the soil surface (mm).

The potential water uptake from any soil layer can be calculated by solving Equation 5.26 for the depth at the top and bottom of the soil layer and taking the difference:

$$w_{up,ly} = w_{up,zl} - w_{up,zu} \qquad (5.27)$$

where $w_{up,ly}$ is the potential water uptake for soil layer *ly* (mm H_2O), $w_{up,zl}$ is the potential water uptake for the profile at the lower boundary of the soil layer (mm H_2O), and $w_{up,zu}$ is the potential water uptake for the profile at the upper boundary of the soil layer (mm H_2O).

Since root density is greatest near the soil surface and decreases with depth, the water uptake from the upper layers is assumed to be much greater than that in the lower layers. The water-use distribution parameter, β_w, is set to 10 in this formulation. With this value, 50% of the water uptake will occur in the upper 6% of the root zone.

The amount of water uptake that occurs on a given day is a function of the amount of water required for the plant for transpiration, E_t, and the amount of water available in the soil, SW (mm H_2O). Equations 5.26 and 5.27 calculate potential water uptake solely as a function of water demand for transpiration and the depth distribution defined in Equation 5.26. Within this formulation, the plant dynamics module modifies the initial potential water uptake from a given soil layer to reflect soil water availability in the following ways.

If the upper layers in the soil profile do not contain enough water to meet the potential water uptake, calculated in Equation 5.27, users may allow lower layers to compensate. The equation used to calculate the adjusted potential water uptake is:

$$w'_{up,ly} = w_{up,ly} + w_{demand} \cdot epco \qquad (5.28)$$

where $w'_{up,ly}$ is the adjusted potential water uptake for layer *ly* (mm H_2O), w_{demand} is the water uptake demand not met by overlying soil layers (mm H_2O), and *epco* is the plant uptake compensation factor.

The plant uptake compensation factor can range from 0.01 to 1.00 and is set by the user. As epco approaches 1.0, the model allows more of the water uptake demand to be met by lower layers in the soil. As epco approaches 0.0, the model allows less variation from the depth distribution, described in Equation 5.26, to take place.

As the water content of the soil decreases, the water in the soil is held more and more tightly by the soil particles and it becomes increasingly difficult for the plant to extract water from the soil. To reflect the decrease in the efficiency of the plant in extracting water from dryer soils, the potential water uptake is modified using the following equations:

$$w''_{up,ly} = w'_{up,ly} * \exp\left[5\left(\frac{SW_{ly}}{(0.25AWC_{ly})} - 1\right)\right] \qquad SW_{ly} < (0.25AWC_{ly}) \qquad (5.29a)$$

$$w''_{up,ly} = w'_{up,ly} \qquad SW_{ly} >= (0.25AWC_{ly}) \qquad (5.29b)$$

where $w''_{up,ly}$ is the potential water uptake adjusted for initial soil water content (mm H_2O), SW_{ly} is the amount of water in the soil layer on a given day (mm H_2O), and AWC_{ly} is the available water capacity for layer *ly* (mm H_2O).

The available water capacity is calculated:

$$AWC_{ly} = FC_{ly} - WP_{ly} \qquad (5.30)$$

where FC_{ly} is the water content of layer *ly* at field capacity (mm H_2O), and WP_{ly} is the water content of layer *ly* at wilting point (mm H_2O).

Once the potential water uptake has been modified for soil water conditions, the actual amount of water uptake from the soil layer is calculated:

$$w_{actualup,ly} = \min\left[w''_{up,ly}, \left(SW_{ly} - WP_{ly}\right)\right] \qquad (5.31)$$

where $w_{actualup,ly}$ is the actual water uptake for layer *ly* (mm H_2O).

The total water uptake for the day is calculated:

$$w_{actualup} = \sum_{ly=1}^{n} w_{actualup,ly} \qquad (5.32)$$

where *n* is the number of layers in the soil profile.

The total plant water uptake for the day, calculated with Equation 5.32, is also the actual amount of transpiration that occurs on the day.

$$E_{t,act} = w_{actualup} \qquad (5.33)$$

Nutrient Uptake by Plants

The current formulations account for nitrogen and phosphorus uptake by plants. The simulation of nitrogen and phosphorus uptake and partitioning to plants follows the approach of the EPIC model. The approach allows simulation of changing allocations of nitrogen and phosphorus based on availability and demand.

Nitrogen Uptake

Nitrogen is taken into plant roots from soil solution as nitrate (NO_3). Ammonium (NH_4) can also be used as a source of Nitrogen, but must first be converted to nitrate by soil micro-organisms. Plant nitrogen uptake is controlled by the plant nitrogen equation. The plant nitrogen equation calculates the fraction of nitrogen in the plant biomass as a function of growth stage given optimal growing conditions:

$$fr_N = \left(fr_{N,1} - fr_{N,3}\right)\left[1 - \frac{fr_{PHU}}{fr_{PHU} + \exp\left(n_1 - n_2 fr_{PHU}\right)}\right] + fr_{N,3} \qquad (5.34)$$

where fr_N is the fraction of nitrogen in the plant biomass on a given day, $fr_{N\,1}$ is the normal fraction of nitrogen in the plant biomass at emergence, $fr_{N,3}$ is the normal fraction of nitrogen in the plant biomass at maturity, and n_1 and n_2 are shape coefficients calculated by solving Equation 5.34 using two known points ($\mathrm{fr}_{N,2}$, $\mathrm{fr}_{PHU,50\%}$) and ($\mathrm{fr}_{N,3}$, $\mathrm{fr}_{PHU,100\%}$):

$$n_1 = \ln\left[\frac{fr_{PHU,50\%}}{1 - \frac{\left(fr_{N,2} - fr_{N,3}\right)}{\left(fr_{N,1} - fr_{N,3}\right)}} - fr_{PHU,50\%}\right] + n_2 fr_{PHU,50\%} \qquad (5.35a)$$

$$n_2 = \frac{\left(\ln\left[\frac{fr_{PHU,50\%}}{1 - \frac{\left(fr_{N,2} - fr_{N,3}\right)}{\left(fr_{N,1} - fr_{N,3}\right)}} - fr_{PHU,50\%}\right] - \ln\left[\frac{fr_{PHU,100\%}}{1 - \frac{\left(fr_{N,\sim 3} - fr_{N,3}\right)}{\left(fr_{N,1} - fr_{N,3}\right)}} - fr_{PHU,100\%}\right]\right)}{fr_{PHU,100\%} - fr_{PHU,50\%}} \qquad (5.35b)$$

where $fr_{PHU,50\%}$ is the fraction of potential heat units accumulated for the plant at 50% maturity ($\mathrm{fr}_{PHU,50\%} = 0.50$), and $fr_{PHU,100\%}$ is the fraction of potential heat units accumulated for the plant at maturity ($\mathrm{fr}_{PHU,100\%} = 1.0$). The normal fraction of nitrogen in the plant biomass near maturity is used in Equation 5.35b to ensure that the denominator term, $\left(1-\frac{\left(fr_{N,\sim 3}-fr_{N,3}\right)}{\left(fr_{N,1}-fr_{N,3}\right)}\right)$, does not equal 1. The formulation assumes $(fr_{N,\sim 3} - fr_{N,3}) = 0.00001$.

To determine the mass of nitrogen that should be stored in the plant biomass on a given day the nitrogen fraction is multiplied by the total plant biomass:

$$bio_{N,opt} = fr_N \cdot bio \tag{5.36}$$

The plant nitrogen demand for a given day is determined by taking the difference between the nitrogen content of the plant biomass expected for the plant's growth stage and the actual nitrogen content:

$$N_{up} = bio_{N,opt} - bio_N \tag{5.37}$$

where N_{up} is the potential nitrogen uptake (kg N/ha).

The depth distribution of nitrogen uptake is calculated with the equation:

$$N_{up,z} = \frac{N_{up}}{\left[1-\exp\left(-\beta_n\right)\right]}\left[1-\exp\left(-\beta_n \frac{z}{z_{root}}\right)\right] \tag{5.38}$$

where $N_{up,z}$ is the potential nitrogen uptake from the soil surface to depth z (kg N/ha), and β_n is the nitrogen uptake distribution parameter.

The potential nitrogen uptake for a soil layer is calculated by solving equation 5.38 for the depth at the upper and lower boundaries of the soil layer and taking the difference:

$$N_{up,ly} = N_{up,zl} - N_{up,zu} \tag{5.39}$$

where $N_{up,ly}$ is the potential nitrogen uptake for layer ly (kg N/ha), $N_{up,zl}$ is the potential nitrogen uptake from the soil surface to the lower boundary of the soil layer (kg N/ha), and $N_{up,zu}$ is the potential nitrogen uptake from the soil surface to the upper boundary of the soil layer (kg N/ha).

Since root density is greatest near the surface nitrogen uptake in the upper portion of the soil will be greater than in the lower portion. The depth distribution of nitrogen uptake is controlled by β_n, the nitrogen uptake distribution parameter, a variable users are allowed to adjust.

Nitrogen removed from the soil by plants is taken from the nitrate pool. The importance of the nitrogen uptake distribution parameter lies in its control over the maximum amount of nitrate removed from the upper layers. Because the top 10 mm of the soil profile interacts with surface runoff, the nitrogen uptake distribution parameter will influence the amount of nitrate available for transport in surface runoff. This formulation allows lower layers in the root zone to fully compensate for lack of nitrate in the upper layers, so there should not be significant changes in nitrogen stress with variation in the value used for β_n.

The actual amount of nitrogen removed from a soil layer is calculated:

$$N_{actualup,ly} = \min\left[N_{up,ly} + N_{demand}, NO3_{ly}\right] \qquad (5.40)$$

where $N_{actualup,ly}$ is the actual nitrogen uptake for layer ly (kg N/ha), N_{demand} is the nitrogen uptake demand not met by overlying soil layers (kg N/ha), and $NO3_{ly}$ is the nitrate content of soil layer ly (kg NO_3-N/ha).

Nitrogen Fixation

If nitrate levels in the root zone are insufficient to meet the demand of a legume, this formulation allows the plant to obtain additional nitrogen through nitrogen fixation. Nitrogen fixation is calculated as a function of soil water, soil nitrate content, and growth stage of the plant:

$$N_{fix} = N_{demand} f_{gr} \cdot \min\left(f_{sw}, f_{NO3}, 1\right) \qquad (5.41)$$

where N_{fix} is the amount of nitrogen added to the plant biomass by fixation (kg N/ha), f_{gr} is the growth stage factor (0.0 - 1.0), f_{sw} is the soil water factor (0.0 - 1.0), and f_{NO3} is the soil nitrate factor (0.0 - 1.0). The maximum amount of nitrogen that can be fixed by the plant on a given day is N_{demand}.

Growth stage exerts the greatest impact on the ability of the plant to fix nitrogen. The growth stage factor is calculated:

$$f_{gr} = 0.0 \qquad fr_{PHU} <= 0.15 \qquad (5.42a)$$

$$f_{gr} = 6.67 fr_{PHU} - 1.0 \qquad 0.15 < fr_{PHU} <= 0.30 \qquad (5.42b)$$

$$f_{gr} = 1.0 \qquad 0.30 < fr_{PHU} <= 0.55 \qquad (5.42c)$$

$f_{gr} = 3.75 - 5.0 fr_{PHU}$ $\quad 0.55 < fr_{PHU} <= 0.75 \quad$ (5.42d)

$f_{gr} = 0.0$ $\quad fr_{PHU} > 0.75 \quad$ (5.42e)

The soil nitrate factor inhibits nitrogen fixation as the presence of nitrate in the soil goes up. The soil nitrate factor is calculated:

$f_{NO3} = 1.0$ $\quad NO3 <= 100 \quad$ (5.43a)

$f_{NO3} = 1.5 - 0.0005 NO3$ $\quad 100 < NO3 <= 300 \quad$ (5.43b)

$f_{NO3} = 0.0$ $\quad NO3 > 300 \quad$ (5.43c)

where *NO3* is the nitrate content of the soil profile (kg NO_3-N/ha).

The soil water factor is calculated:

$$f_{sw} = \frac{SW}{0.85\theta_{fc}} \qquad (5.44)$$

where SW is the amount of water in the soil profile (mm H_2O) and θ_{fc} is the water content of the soil profile at field capacity (mm H_2O).

Phosphorus Uptake

Phosphorus is an important plant macronutrient, making up about 0.2% of a plant's dry weight. It is a component of key molecules such as nucleic acids, phospholipids, and ATP, and, consequently, plants cannot grow without a reliable supply of this nutrient. Plant phosphorus uptake is controlled by the plant phosphorus equation. The plant phosphorus equation calculates the fraction of phosphorus in the plant biomass as a function of growth stage given optimal growing conditions:

$$fr_P = \left(fr_{P,1} - fr_{P,3}\right)\left[1 - \frac{fr_{PHU}}{fr_{PHU} + \exp\left(p_1 - p_2 * fr_{PHU}\right)}\right] + fr_{P,3} \qquad (5.45)$$

where fr_P is the fraction of phosphorus in the plant biomass on a given day, $fr_{P,1}$ is the normal fraction of phosphorus in the plant biomass at emergence, $fr_{P,3}$ is the normal fraction of phosphorus in the plant biomass at maturity, and p_1 and p_2 are shape coefficients calculated by solving Equation 5.45 using two known points ($fr_{P,2}$, $fr_{PHU,50\%}$) and ($fr_{P,3}$, $fr_{PHU,100\%}$):

$$p_1 = \ln\left[\frac{fr_{PHU,50\%}}{1 - \frac{(fr_{P,2} - fr_{P,3})}{(fr_{P,1} - fr_{P,3})}} - fr_{PHU,50\%} \right] + p_2 \cdot fr_{PHU,50\%} \qquad (5.46a)$$

$$p_2 = \frac{\left(\ln\left[\frac{fr_{PHU,50\%}}{1 - \frac{(fr_{P,2} - fr_{P,3})}{(fr_{P,1} - fr_{P,3})}} - fr_{PHU,50\%} \right] - \ln\left[\frac{fr_{PHU,100\%}}{1 - \frac{(fr_{P,\sim 3} - fr_{P,3})}{(fr_{P,1} - fr_{P,3})}} - fr_{PHU,100\%} \right] \right)}{fr_{PHU,100\%} - fr_{PHU,50\%}} \qquad (5.46b)$$

where the normal fraction of phosphorus in the plant biomass near maturity is used in Equation 5.46b to ensure that the denominator term, $\left(1 - \frac{(fr_{P,\sim 3} - fr_{P,3})}{(fr_{P,1} - fr_{P,3})}\right)$, does not equal 1. The formulation assumes $(fr_{P,\sim 3} - fr_{P,3}) = 0.00001$.

To determine the mass of phosphorus that should be stored in the plant biomass for the growth stage, the phosphorus fraction is multiplied by the total plant biomass:

$$bio_{P,opt} = fr_P \cdot bio \qquad (5.47)$$

The plant nitrogen demand for a given day is a function of the difference between the phosphorus content of the plant biomass expected for the plant's growth stage and the actual phosphorus content:

$$P_{up} = 1.5(bio_{P,opt} - bio_P) \qquad (5.48)$$

where P_{up} is the potential phosphorus uptake (kg P/ha). The difference between the phosphorus content of the plant biomass expected for the plant's growth stage and the actual phosphorus content is multiplied by 1.5 to simulate luxury phosphorus uptake, the continued uptake beyond what is required for immediate growth.

The depth distribution of phosphorus uptake is calculated with the equation:

$$P_{up,z} = \frac{P_{up}}{\left[1-\exp\left(-\beta_p\right)\right]}\left[1-\exp\left(-\beta_p \frac{z}{z_{root}}\right)\right] \qquad (5.49)$$

where $P_{up,z}$ is the potential phosphorus uptake from the soil surface to depth z (kg P/ha), and β_p is the phosphorus uptake distribution parameter.

The potential phosphorus uptake for a soil layer is calculated by solving Equation 5.49 for the depth at the upper and lower boundaries of the soil layer and taking the difference:

$$P_{up,ly} = P_{up,zl} - P_{up,zu} \qquad (5.50)$$

where $P_{up,ly}$ is the potential phosphorus uptake for layer ly (kg P/ha), $P_{up,zl}$ is the potential phosphorus uptake from the soil surface to the lower boundary of the soil layer (kg P/ha), and $P_{up,zu}$ is the potential phosphorus uptake from the soil surface to the upper boundary of the soil layer (kg P/ha).

Root density is greatest near the surface, and phosphorus uptake in the upper portion of the soil will be greater than in the lower portion. The depth distribution of phosphorus uptake is controlled by β_p, the phosphorus uptake distribution parameter, a variable users are allowed to adjust.

Phosphorus removed from the soil by plants is taken from the solution phosphorus pool. The importance of the phosphorus uptake distribution parameter lies in its control over the maximum amount of solution P removed from the upper layers. Because the top 10 mm of the soil profile interacts with surface runoff, the phosphorus uptake distribution parameter will influence the amount of labile phosphorus available for transport in surface runoff. This formulation allows lower layers in the root zone to fully compensate for lack of solution P in the upper layers, so there should not be significant changes in phosphorus stress with variation in the value used for β_p.

The actual amount of phosphorus removed from a soil layer is calculated:

$$P_{actualup,ly} = \min\left(P_{up,ly} + P_{demand}, P_{solution,ly}\right) \qquad (5.51)$$

where $P_{actualup,ly}$ is the actual phosphorus uptake for layer ly (kg P/ha), P_{demand} is the phosphorus uptake demand not met by overlying soil layers (kg P/ha), and $P_{solution,ly}$ is the phosphorus content of the soil solution in layer ly (kg P/ha).

Crop Yield and Nutrients Removed

When a harvest or harvest/kill operation is performed, a portion of the plant biomass is removed from the land surface as yield. The nutrients and plant material contained in the yield are assumed to be lost from the system (i.e., watershed) and will not be added to residue and organic nutrient pools in the soil with the remainder of the plant material. In contrast, a kill operation converts all biomass to residue.

Crop Yield

The crop yield is calculated as:

$$yld = bio_{ag} \cdot HI \qquad \text{HI} <= 1.0 \qquad (5.52a)$$

$$yld = bio \cdot \left(1 - \frac{1}{(1 + HI)}\right) \qquad \text{HI} > 1.0 \qquad (5.52b)$$

where *yld* is the crop yield (kg/ha), *HI* is potential harvest index, and bio_{ag} is the aboveground biomass on the day of harvest (kg/ha).

The aboveground biomass is calculated:

$$bio_{ag} = (1 - fr_{root})bio \qquad (5.53)$$

where fr_{root} is the fraction of the total biomass in the roots the day of harvest.

Potential harvest index

The fraction of the above ground plant dry biomass removed as dry economic yield is called the harvest index. For the majority of crops, the harvest index will be between 0.0 and 1.0. However, plants whose roots are harvested, such as sweet potatoes, may have a harvest index greater than 1.0.

The economic yield of most commercial crops is the reproductive portion of the plant. Decades of crop breeding have lead to cultivars and hybrids having maximized harvest indices. Often, the harvest index is relatively stable across a range of environmental conditions.

The harvest index, for each day of the plant's growing season, uses the following equation:

$$HI = HI_{opt} \frac{100 fr_{PHU}}{100 fr_{PHU} + \exp(11.1 - 10 fr_{PHU})} \tag{5.54}$$

where HI is the potential harvest index for a given day and HI_{opt} is the potential harvest index for the plant at maturity given ideal growing conditions.

Actual harvest index

The harvest index is affected by water deficit; actual harvest index is calculated using the following equation:

$$HI_{act} = (HI - HI_{\min}) \frac{\gamma_{wu}}{\gamma_{wu} + \exp(6.13 - 0.833\gamma_{wu})} + HI_{\min} \tag{5.55}$$

where HI_{act} is the actual harvest index, HI_{min} is the harvest index for the plant in drought conditions and represents the minimum harvest index allowed for the plant, and γ_{wu} is the water deficiency factor.

The water deficiency factor is calculated:

$$\gamma_{wu} = 100 * \frac{\sum_{i=1}^{m} E_a}{\sum_{i=1}^{m} E_o} \tag{5.56}$$

where E_a is the actual evapotranspiration, E_o is the potential evapotranspiration, and m is the day of harvest if the plant is harvested before it reaches maturity or the last day of the growing season if the plant is harvested after it reaches maturity.

Nutrients Removed

The amount of nutrients removed in the yield is calculated as:

$$N_{yld} = fr_{N,yld} \cdot yld \tag{5.57a}$$

$$P_{yld} = fr_{P,yld} \cdot yld \tag{5.57b}$$

where N_{yld} is the amount of nitrogen removed in the yield (kg N/ha), P_{yld} is the amount of phosphorus removed in the yield (kg P/ha), $fr_{N,yld}$ is the fraction of nitrogen in the yield, and $fr_{P,yld}$ is the fraction of phosphorus in the yield (kg/ha).

If the harvest index override is used in the harvest only operation, the formulation assumes that a significant portion of the plant biomass is being removed in addition to the seed. Therefore, instead of using the nitrogen and phosphorus yield fractions from the plant growth database, the formulation uses the total biomass nitrogen and phosphorus fractions to determine the amount of nitrogen and phosphorus removed:

$$N_{yld} = fr_N \cdot yld \tag{5.58a}$$

$$P_{yld} = fr_P \cdot yld \tag{5.58b}$$

6 Model Validation Studies

In developing any numerical model, validation of the process descriptions is very important if the model is to be used in a predictive mode. With that in mind two demonstration projects are currently underway. The first is the Eau Galle watershed located in Wisconsin and the second is the Upper Auglaize Watershed located in Ohio. In both cases model results were not completed in time for this publication. This report will give a general description of the demonstration sites and goals of the studies. Results will be published later in companion technical notes.

Eau Galle Watershed Demonstration

The Eau Galle River watershed encompasses a 402 km^2 area in northwest Wisconsin, Figure 3 (Downer, 2007).

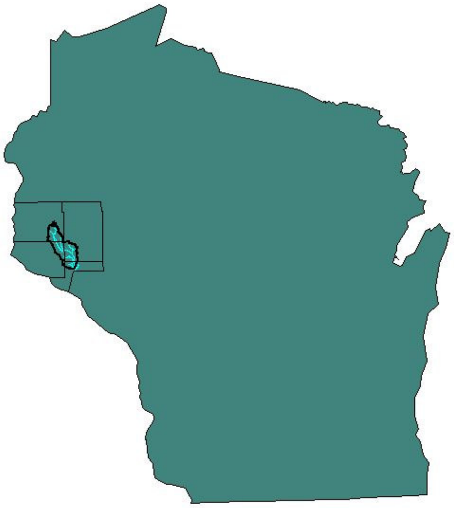

Figure 3 – Location of Eau Galle River watershed

While the larger basin is important, the lower portion of the basin, Figure 4, is relatively data poor. The data, particularly rainfall, are not sufficient for the testing of new model developments. The upper portion of the watershed, that portion above Spring Valley Dam, Figure 5, has been the subject of intensive past studies, and compared to the lower portion of the watershed, is relatively data rich. This

$103\ km^2$ sub-watershed was selected to demonstrate the NSM model, as well as other features in the GSSHA model.

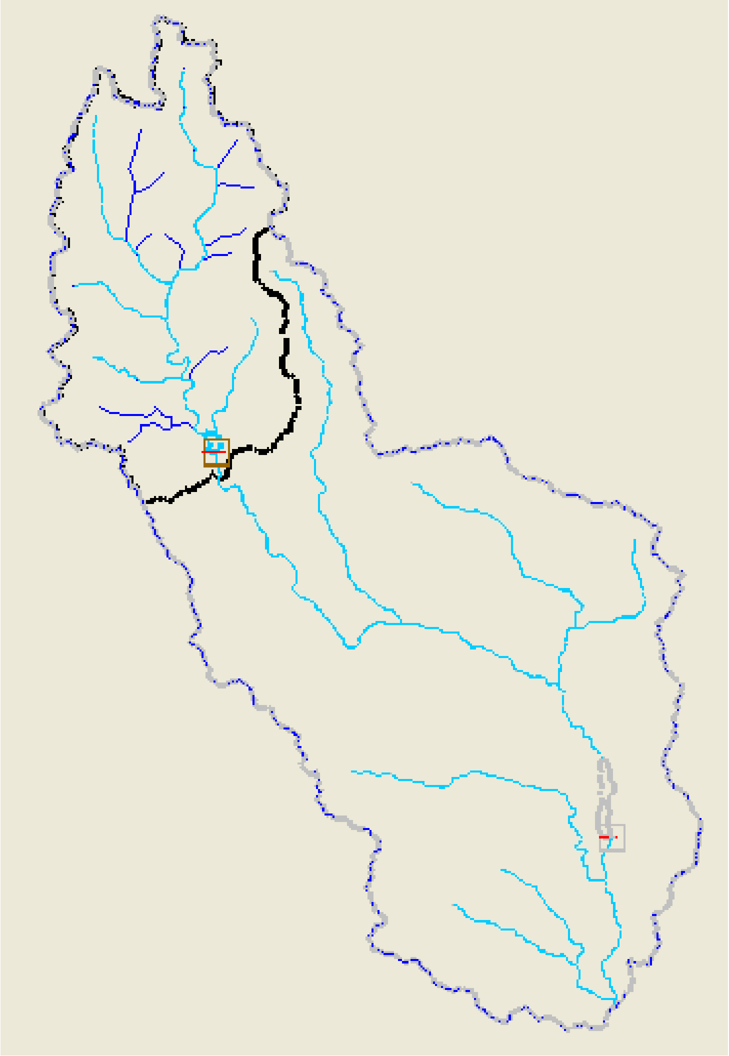

Figure 4 – Spring Valley Dam watershed.

In addition the Spring Valley Dam watershed has these important features:

- Reservoir with controlled discharge
- Mixed hydrology basin with contributions from surface and subsurface
- Agricultural basin with diffuse nutrient sources
- Dentritic stream network

With the observed data and complex features found within the Upper Eau Galle Watershed this study area is ideal for testing, validating and further developing the flow, sediment, and nutrient algorithms found within GSSHA and NSM.

Upper Auglaize Watershed Demonstration

The Upper Auglaize Watershed is located in portions of Auglaize, Allen, Putnam, and VanWert counties in the southern portion of the Maumee River Basin. The watershed encompasses 211,956 acres (~330 mi^2) upstream of the USGS Fort Jennings gaging station, Figure 5. Land use is predominantly agricultural with 74.2% cropland, 10.8% grassland, 6.2% woodland, and 8.8% urban and other landuses. Blount and Pewamo are major soil types in the watershed. These soils are characterized as somewhat poorly to very poorly drained with moderately slow permeability. Farm fields in the watershed are extensively tile drained and the area has a very extensive network of man-made or man-altered drainage ditches. Common conservation practices applied in the watershed include grassed waterways, tile and surface drainage, conservation-tillage and no-tillage, grass filter strips, and erosion control structures. Soils are among the most productive in Ohio and fields not still in woodland or USDA set-aside cover are intensively farmed. At the present time, no-tillage (no-till) is practiced on 51% of the cropped fields and mulch tillage on 17%. Most natural fencerows have been removed. There is a modest amount of livestock in the watershed, most of which is in confined feeding setups with very few animals on pasture.

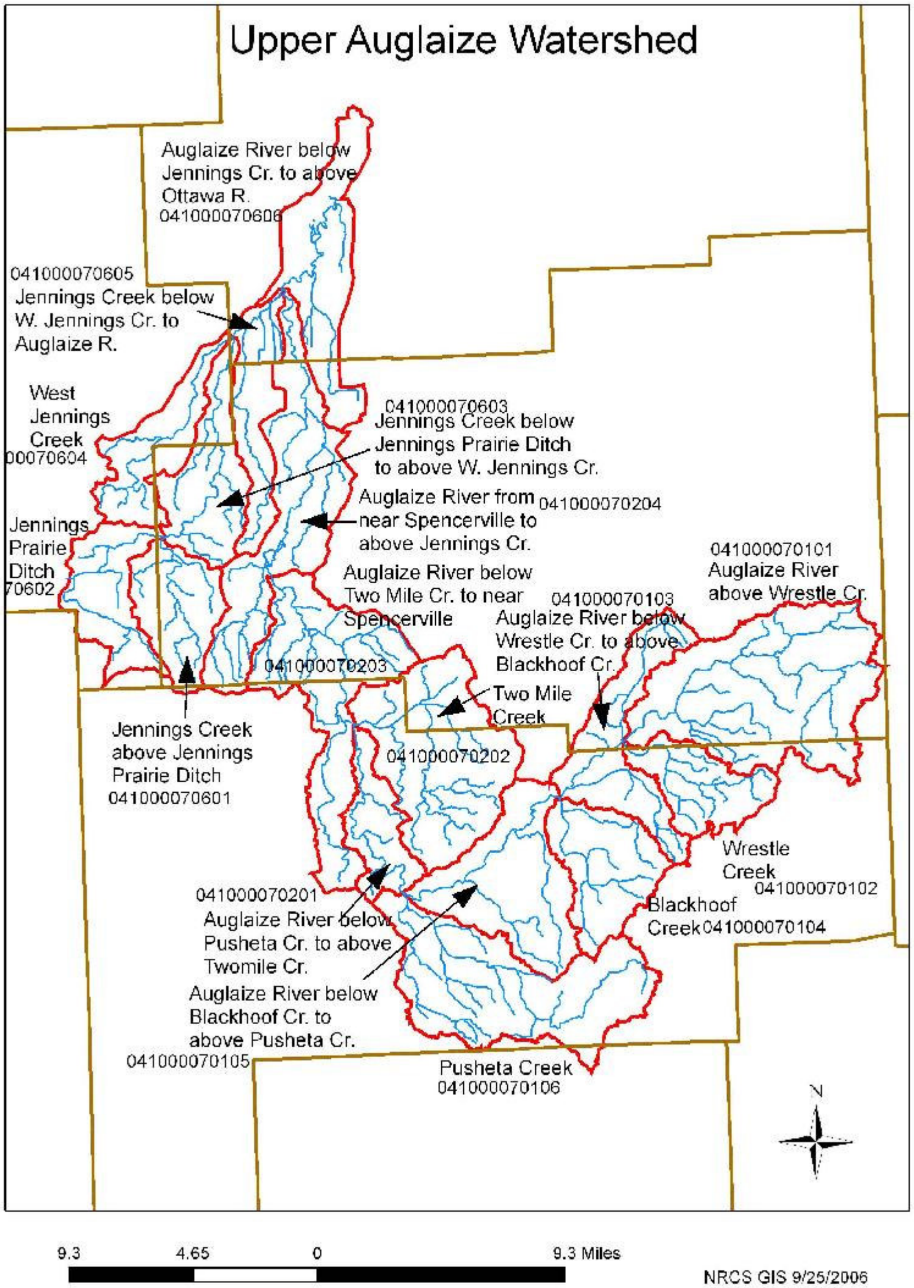

Figure 5 - Upper Auglaize Watershed (Bingner, 2005)

The overall purpose of the Upper Auglaize Watershed Demonstration is targeted at performing the monitoring and modeling design needed to create both: 1) the *linkage* between the established, recognized edge-of –field tool, DRAINMOD and established subwatershed and watershed models and 2) the *capability*, at the subwatershed and watershed scale to reliably predict the transport of agricultural loadings from the edge-of-field to both subwatershed and watershed outlets. This missing capability may contain the understanding of system response we currently lack to effectively predict, track and manage hypoxic conditions in receiving water bodies

The modeling phase of the project will involve the development of enhanced, integrated modeling components for surface/subsurface transport of sediments and nutrients from agricultural fields to the outlet of the watershed. This component of the study is envisioned as a multi-year effort (3 years) and features the integration of state-of-the-art monitoring, modeling and remote sensing components.

Summary

Within this report, the major development efforts since the release of NSMv1.0 have been discussed. These improvements were in the area of: 1) partitioning of nutrients (dissolved and adsorbed) within surface runoff; 2) mass transfer of nutrients between the soils and overlying water column; 3) erosion and sedimentation of particulate nutrients; and 4) soil plant dynamics.

Nutrients at or near the soil surface can be transformed to overland flow in solution form by the mixing of rainwater with soil solution. A rate-limited mass transfer at the soil overland flow interface controls the dissolved nutrient transfer from soil solution to overland flow, once formed. The mass transfer coefficient will be affected by many factors among which are the characteristics of the rain drops, the overland flow, and nutrient characteristics. The predictions of these variables, together with nutrient transport in the surface runoff, are needed to be validated with the measured data at the field scale.

In regards to the soil plant dynamics capabilities within NSM, the EPIC formulations do appear to provide realistic responses for simple annual based systems. It is necessarily simple for use with the available datasets and should be improved by addition of plant growth processes with nutrient cycling. Further development of this module for a more detailed treatment of plant water uptake and associated nutrient interactions is needed. Attention to refinement of links between soil plant dynamics and hydrological processes is also required.

As research continues, improved understanding of nutrient process descriptions and new capabilities will be developed and as such will be integrated into the NSM. Future releases of NSM will include: 1) improved nutrient kinetics for channels; 2) improved soil plant dynamics (EDYS sub-module); 3) inclusion of carbon cycle modules for soils and overland flow; and 4) improved nitrogen and phosphorus kinetics for soils and overland flow.

References

Ahuja, L.R. and Lehman, O.R. (1983). "The extent and nature of rainfall-soil interaction in the release of soluble chemicals to runoff." *J. Environ. Qual.* 12: 34-40.

Bingner, Ron, et al (2005). "Upper Auglaize Watershed AGNPS Modeling Project Final Report", prepared for the U.S. Army Corps of Engineers - Buffalo District, Buffalo, NY.

Burt, T.P., A.L. Heathwaite, and S.T. Trudgill. (1993). *Nitrate: Processes, Patterns and Management*. Chapters 5 & 10, John Wiley & Sons, Inc., New York.

Chapra, S.C. (1997). *Surface water-quality modeling.* The McGraw-Hill Companies, Inc.

Choy, B., and Reible, D.D. (1999). "Contaminant transport in soils and sediments: Mathematicalanalysis." Report to the Hazardous Substance Research Center (S&SW), Louisiana State University, Baton Rouge, LA.

Downer, Charles W. (2007). "Demonstration of GSSHA hydrology and sediment, at the Eau Galle Watershed near Spring Valley, WI.", ERDC/CHL TN (In Review), Vicksburg, MS.

Gao, B., M.T. Walter, T.S. Steenhuis, W.L. Hogarth, and J.-Y. Parlange (2004). "Rainfall induced chemical transport from soil to runoff: theory and experiments." *J. Hydrol.* 295(1-4): 291-304.

Fischer et al., H.B. Fischer, E.J. List, R.C.Y. Koh, J. Imberger and N.H. (1979). Brooks, *Mixing in Inland and Coastal Waters*, Academic Press, New York.

Foster G.R., Meyer L.D., and Onstad C.A. (1977). "A runoff erosivity factor and variable slope length exponents for soil loss estimates." *Trans. ASAE* 20: 683-687.

Johnson, B.E. and T.K. Gerald (2006) "Development of a distributed nutrient sub-model (NSM Version 1.0) for watersheds –kinetic process descriptions." ERDC/EL TR-06-12, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

Jones, C.A. (1985). *C-4 Grasses and Cereals*. John Wiley & Sons, Inc., New York.

Jones, C.A., Bland,W.L., Ritchie, J.T., and Williams, J.R. (1991). "Simulation of root growth." In: Hanks, J., Ritchie, J.T. (Eds.), *Modeling Plant and Soil Systems, Agronomy No. 31* ASA, CSSA. SSSA Publ., Madison, WI, pp. 91–123.

Kookana, R.S., Baskaran, S, and Naidu, R. (1998). "Pesticide fate and behaviour in Australian soils in relation to contamination and management of soil and water: a review." *Australian Journal of Soil Research* 36: 715–764.

McCree, K.J. (1972). The action spectrum, absorption and quantum yield of photosynthesis in crop plants. *Agric. Met.* 9: 191-216.

Monteith, J.L. (1972). Solar radiation and productivity in tropical ecosystems. *J. Appl. Ecol.* 9: 747-766.

Monteith, J.L. (1977). Climate and the efficiency of crop production in Britian. *Phil. Trans. Res. Soc.* London Ser. B 281: 277-329.

Neitsch, S.L., J.G. Arnold, J.R. Kiniry, J.R. Williams, K.W. King. (2002). "Soil and water assessment tool theoretical documentation, Version 2000." Grassland, Soil, and Water Research Laboratory, Agricultural Research Service, Temple, TX.

Smith, R.E., Goodrich, D. and Quinton, J.N. (1995). 'Dynamic distributed simulation of watershed erosion: the KINEROS2 and EUROSEM models.' *J. Soil Water Conserv.* 50: 517–520.

Snyder, I.K. and Woolhiser, D.A. (1985). "Effects of infiltration on chemical transport into overland flow." *Trans. ASAE* 28: 1450-1457.

Stockle, C.O. and J.R. Kiniry. (1990). Variability in crop radiation-use efficiency associated with vapor-pressure deficit. *Field Crops Res.* 25: 171-181.

Stockle, C.O., J.R. Williams, N.J. Rosenberg, and C.A. Jones. (1992). A method for estimating the direct and climatic effects of rising atmospheric carbon dioxide on growth and yield of crops: Part 1—Modification of the EPIC model for climate change analysis. *Agricultural Systems* 38: 225-238.

Taskinen, A. and Bruen, M. (2007). "Incremental distributed modelling investigation in a small agricultural catchment: 2. Erosion and phosphorus transport." *Hydrological Processes* 21 (1): 92-102.

Wallach, R., W.A. Jury, and W.F. Spencer (1988). "Transfer of chemicals from soil solution to surface runoff: a diffusion-based model." *Soil Sci. Soc. Am. J.* 52(3): 612-618.

Wallach, R., W.A. Jury, and W.F. Spencer (1989). "The concept of convective mass transfer for prediction of surface-runoff pollution by soil surface applied chemicals." *Trans. ASAE* 32(3): 906-912.

Williams, J.R., C.A. Jones, and P.T. Dyke (1984). "A modeling approach to determining the relationship between erosion and soil productivity." *Trans. ASAE* 27 (1):129-144.

Watson, D.J. (1947). "Comparative physiological studies on the growth of field crops. 1. Variation in net assimilation rate and leaf area index between species and varieties and within and between years." *Ann. Bot. N.S.* 11:41-76.

Zhang, X.C., Norton, D., and Nearing, M.A. (1997). "Chemical transfer from soil solution to surface runoff." *Water Resour. Res.* 33 (4): 809–815.