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SIMULATING PROCESSES IN NONPOINT SOURCE POLLUTION

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ABSTRACT

The paper describes development of a mathematical model to evaluate nonpoint pollution from diffuse agricultural and forestry sources. Although the model includes numerous physical and chemical processes, a generalized flow chart is used to present the entire system along with more detailed components. The nitrogen cycling and pesticide elements of the chemistry components are presented. The interactions of complex processes are described relative to climate, soil, and agricultural management practices.

1 INTRODUCTION

In 1978, approximately 50 engineers and scientists in the U. S. Department of Agriculture, Agricultural Research Service (USDA-ARS) met to plan the strategy for developing a mathematical model to assess nonpoint pollution from diffuse agricultural sources. A generalized flow chart was drafted to give a focus to all the pieces representing the major components. Also, the flow chart provided a perspective for how the contribution from each scientist fitted into the whole system. The **CREAMS** model [Chemicals, Runoff, and Erosion from Agricultural Management Systems] for field-size areas (Knisel, 1980) evolved from the group, and its success with only minor modification to input and micro-basing is attested by its continued use and requests 12 years after publication. The flow chart was instrumental in maintaining focus during the development process, and it became a part of the publication cover. The flow-chart is reproduced here as figure 1 for reference purposes. Although **CREAMS** was primarily a surface-response edge-of-field loading model, some root-zone processes were included as well. The flow chart was sufficiently general to include both surface and subsurface processes.

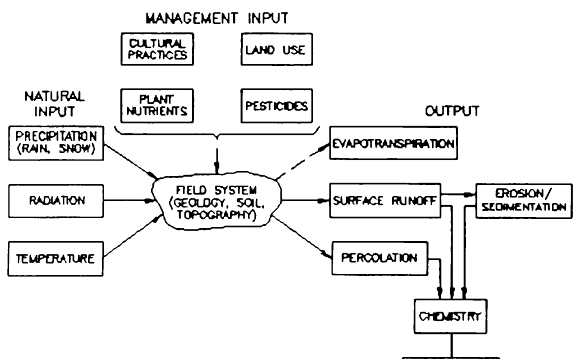

Figure 1: Schematic Representation of the Physical System for the **CREAMS** Model

The **GLEAMS** model [Groundwater Loading Effects of Agricultural Management Systems] (Leonard et al., 1987) was developed as an extension of **CREAMS** to consider the vertical flux of pesticides, and more recently, to include a more complete plant nutrient component (Knisel et al., 1992). **GLEAMS** simulates surface response similar to that of **CREAMS** but also includes root zone processes to give bottom-of-root-zone loadings as well. The generalized flow chart continued to serve the same function of major components on which to build the necessary elements and processes.

The purpose of this paper is to describe the approaches in formulating the complex interactions of the physical and chemical processes that affect nonpoint source pollution. Process formulations are not included.

2 MODEL DESCRIPTION

There were three basic components in the **CREAMS** model: (1) hydrology, (2) erosion/sediment yield, and (3) chemistry. Chemistry actually included two parts: (a) pesticides and (b) plant nutrients. Although there are a number of similarities between the two parts, they are distinctly different, and **GLEAMS** is considered to include four components--hydrology, erosion, pesticides, and plant nutrients. The more obvious differences are: all of the pesticides, including metabolites, are non-conservative and degrade as a function of time, the rate and pathway being compound-specific, whereas only nitrate-nitrogen is non-conservative (denitrification); ammonium-nitrogen may be transformed into nitrate-nitrogen; ammonium and phosphorus mineralize from organic matter; precipitation contains nitrogen, but is not considered to contain significant concentrations of pesticides. This separation is not important in this presentation--only the processes which distinguish themselves. A very brief description of each component is given as well as the climatic and management inputs to the system. The physical field is also defined in general terms.

2.1 Climate

Climate is the driver of the system. Precipitation, in the form or snow or rainfall, radiation, and temperature are the inputs to the system. Not only is climate the driving force, it modifies many of the processes, such as nutrient mineralization rates and infiltration of snowmelt on frozen soils. Also, climate may be a controlling mechanism for management practices, such as crops than can be grown and irrigation needed for sustained production.

The time step in the **GLEAMS** model is one day. Daily precipitation and daily or monthly temperature, and monthly radiation are input to the models. Monthly data are fitted with Fourier series to determine the coefficients for interpolating daily values. Mean daily temperature is used to determine if precipitation on a day is in the form of rainfall or snow. Snow is accumulated over time, and when mean daily air temperature is above freezing, snowmelt is simulated. The resulting rainfall or snowmelt is entered into other physical processes that are formulated and operate in the hydrology component with interactions with other components (Fig. 1).

2.2 Management

Management includes those practices that modify response of the physical system. Crops that are grown within climatic regions, the dates of planting and harvest, dates and rates of fertilization, dates and rates of applicable pesticides, irrigation, chemigation, fertigation, terracing, contour tillage, tillage implement or no-till, residue management, etc., are all practices that may affect field response to climate. These are alternatives that must be assessed in nonpoint source pollution alleviation. A farmer cannot change the soil or the topography of his field, except minimally, or change climate. Thus, management practices can be changed to alter pollutant loads at the edge of the field or bottom of the root zone that may affect quality of groundwater or some off-site water body such as a lake.

2.3 Physical System (Field)

A field is defined in the models as a natural catchment from which surface runoff leaves the area at a single outlet, the soil is homogeneous, it has a single crop at any one time, management is uniform over the area (all terraced, all irrigated, etc.), and precipitation is assumed to be uniform over the area. Soil and precipitation are known to be spatially variable, but for simulation purposes, it is satisfactory to assume uniformity. The field has some topographic signature that includes degree and length of slope, and the topography need not necessarily be uniform over the field, i. e. there may be a wide range of slope steepness and lengths, with or without concentrations of flow into channels.

Without getting into soil morphology or taxonomy, a simplified soil profile within an effective root depth is shown in figure 2. Soil horizons (left side) are described by field survey, and the soil properties are determined from laboratory analyses. Most biological and crop root activity occur in the plow layer, or A_p

horizon, thus the organic matter content and water retention characteristics are generally highest. Also, this is the horizon where most of the plant water and nutrient uptake occur, and the zone where most of the soil evaporation occurs. It is also the horizon that receives rainfall and irrigation water (except in sub-irrigated systems). It is only logical that model computational layers are thinner in the A_p horizon than the lower horizons as shown on the right side of figure 2. However, in the interest of computational time, a maximum of 12 layers was assumed to be sufficient. In the lower soil horizons, the computational layers are allowed to exceed 15 cm thickness to achieve the constraint of 12 layers. With the exception of the surface active layer which is fixed at 1 cm, the remaining computational layers in a soil horizon are of equal thickness.

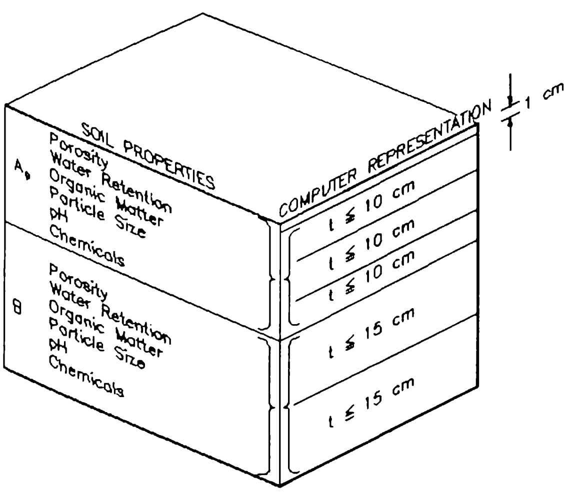

Figure 2: **GLEAMS** Model Representation of Soil Properties by Horizon

Even though characteristics of some soil horizons change gradually from one to the next, they are assumed by the model to be uniform. Each computational layer in a horizon has the same characteristics as the respective horizon. The model determines the layer thickness from the horizon input data and the criteria given above for the layer thicknesses.

2.4 Hydrology

Rainfall, snowmelt, and irrigation are partitioned into surface runoff and infiltration at the soil surface in the hydrology component. Beginning at the surface, if the infiltration volume exceeds the storage capacity of a soil layer, the excess is routed to successively lower layers. If there is excess to what the bottom layer can hold, that excess becomes percolation below the root zone and is considered lost from the system. Percolation represents potential recharge to groundwater, and may contain pesticides and nutrients.

Plant available soil water, i. e. water that can be held between field capacity and wilting point, is acted upon by soil evaporation and plant transpiration in the hydrology component. Evaporation moves water out of the root zone, and moves plant nutrients and pesticides up in the root zone. Transpiration moves water, nutrients, and pesticides into the plant. These processes are calculated daily. The water accounting procedure provides a daily water status in the soil, and when rainfall, snowmelt, or irrigation occur, the available storage is known for partitioning water input into the soil surface. Irrigation can be actuated automatically in the model by user specification of the soil water threshold at which water is to be applied.

The hydrology component also generates crop growth as a function of user-defined growth characteristics (leaf area index), and water and nutrient availability or stress.

The hydrology component also calculates a peak rate of runoff and rainfall energy from daily rainfall amount to be used in the erosion component. Use of these rainfall and runoff characteristics will be described below.

2.5 Erosion

Soil detachment by raindrop impact and sediment transport by runoff are simulated for simple or complex overland flow profiles. Rainfall energy is calculated in the hydrology component as well as the characteristic discharge used to estimate sediment transport capacity. Soil protection from raindrop detachment afforded by the crop canopy and surface residue is a function of management practice, and is simulated in the model. Resistance to flow is a function of management, also, and it, too, is represented in the model to simulate sediment transport capacity.

Soil erodibility, an empirical factor, is a fundamental soil property that is a measure of susceptibility of the soil to detachment by raindrop impact and flowing water. It is a soil-specific characteristic that is a function of soil texture (particle size distribution), soil structure (particle arrangement), organic matter content, and drainage. Management has little affect on soil erodibility over a very small range due to practices that affect organic matter, structure, and drainage.

Field topography, i. e. slope length and steepness, directly influences sediment transport. The **GLEAMS** model considers a representative overland flow profile (slope shape) and channel or concentrated flow characteristics. These features are a part of the physical system described above that affect sediment yield, and are not related to management except over a small range on land-formed sites. Land forming (planing) may be used as a practice to enhance surface drainage or to provide a more uniform water application in basin (flood) or furrow irrigation systems.

Direction of tillage, i. e. up-and-down hill versus on the contour as extremes, affect erosion and sediment transport. Tillage direction is a function of management practices applied by the farmer, for example contour tillage. Contour tillage and residue management, with terraces to break the natural slope length, are resource conservation practices that provide alternative systems for erosion control.

Detached soil particles are routed by particle size through the field delivery system (overland flow and concentrated flow sequences). If transport capacity, estimated from discharge rate calculated in hydrology, is not sufficient to transport the sediment load, deposition is calculated beginning with the largest particles first. The selective transport process results in an enrichment of the finest sediment particles. An enrichment ratio, (ratio of sediment specific surface area to specific surface area of the field soil) is calculated for each erosion event. The enrichment ratio and sediment yield are used in the plant nutrient and pesticide components to calculate the adsorbed chemical transport.

Winter cover crops are management alternatives to provide soil protection during non-crop periods. A winter small grain may be harvested for grain, incorporated into the soil by tillage, or killed with a herbicide in a conservation tillage system. Each practice relates to management alternatives that affect erosion and sediment yield as well as adsorbed chemical transport.

2.6 Pesticides

Pesticides may be applied on the soil surface, applied to a crop canopy, incorporated into a tilled layer of surface soil, or may be injected at some depth below the surface. Method of application depends on the pest to be controlled, chemical characteristics and formulation, and the cropping system. Up to 10 pesticides, with multiple applications each year, can be simulated in a single computer run.

The pesticide component can best be depicted by figure 3 with explanation of the processes involved. Surface-applied, incorporated, and injected pesticides are all considered to be acted upon by the same degradation rates calculated daily. Some of the pesticides that are applied to the crop canopy actually reaches the soil surface and some remains on the plants. The soil fraction is treated just like the surface soil application just discussed. The foliar fraction is subjected to temperature extremes, wind, and radiation, and for most pesticides the dissipation rates from foliage is more rapid than from soil (primarily microbial processes). When rainfall or irrigation occurs, some fraction ranging from 5 to 95% of that remaining on the foliage can be washed off the plant. The washoff fraction is compound dependent. When the canopy storage of water (interception) is exceeded, the pesticide washoff fraction is added to the pesticide mass in the surface 1 cm of soil and is further treated the same as that already in the soil.

The pesticide component calculates the degradation, and amount remaining, for each compound in each computational soil layer each day. The status of pesticides in the surface active 1-cm of soil determines the amount that may be extracted into the runoff stream and the adsorbed fraction that is acted upon by erosion when a runoff-producing event occurs. The extraction into runoff is compound dependent. The concentration of adsorbed pesticide in the surface layer, the sediment yield, and its enrichment of clay and organic matter are used to calculate the pesticide lost with sediment.

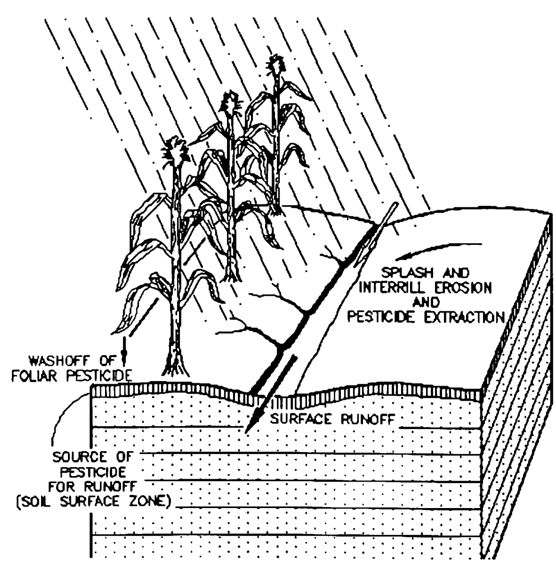

Figure 3: GLEAMS Model Pesticide Component Representation

Pesticides partition between organic carbon (organic matter) and water, and the partitioning coefficient is compound dependent. The water concentration is calculated each day in each computational soil layer. That concentration is used with the soil evaporation calculated in hydrology for the respective layers to estimate the pesticide mass moved into the layer above. Plant transpiration calculated in hydrology and the pesticide concentration in the water of the respective layers are used to estimate plant uptake of pesticides. This daily accounting provides the status of each pesticide on days of rainfall or irrigation. Distribution of pesticides in the root zone is significant in estimating their fate in the environment, either surface or subsurface response.

Management alternatives affecting pesticide fate include selection among recommended EPA-registered compounds to eradicate target pests. Selection of soluble mobile pesticides may reduce surface losses due to infiltration before storm runoff begins, but their movement into the root zone may result in potential problems of groundwater contamination. Both considerations must be addressed simultaneously for complete assessment.

2.7 Plant Nutrients

Nitrogen and phosphorus are the plant nutrients of primary concern in the environment. These cause eutrophication of surface waters, and nitrate-nitrogen in drinking water may be harmful to human health, particularly infants. Therefore, N and P are the only elements considered in the **GLEAMS** nutrient component. The nutrient component was selected for major emphasis in this paper, and more attention is given here for that reason rather than the relative importance of the component.

The nitrogen cycle is shown in figure 4. The processes are shown on the arrows as two-letter symbols: IM = immobilization; AM = ammonification; NI = nitrification; FX = fixation; VL = volatization; DN = denitrification; UP = uptake. Nitrogen losses are shown in figure 4 as well: RO = runoff; SED = sediment; and PERC = percolation. Although they are not shown, erosion/sediment transport accounts for losses of organic nitrogen, and active and stable soil nitrogen.

Figure 4 includes both surface and subsurface processes. For example, rainfall nitrogen is input at the surface; fertilizer and animal waste may be applied on the surface (where volatization of ammonia in animal waste occurs) or may be incorporated into the soil; above-ground crop residue is at the surface but crop roots are in the soil; harvestable yield may be above ground or in the soil (peanuts, potatoes, carrots, etc); uptake occurs within the soil; and fixation occurs from above ground but it assimilates nitrogen in both the above ground and soil parts of legumes.

The phosphorus cycle (figure 5) is simpler than that for nitrogen. The major processes are shown in the figure as two-letter symbols on the arrows: MN = mineralization; IM = immobilization; and UP = uptake. Mineralization is a one-step process, and phosphorus does not volatize nor is it assimilated from the atmosphere. As was the case with nitrogen, losses of phoshporus include: RO = runoff; SED = sediment, and PERC = percolation. Erosion/sediment transport losses of organic P, active soil P, and stable soil P are not shown for the phosphorus cycle.

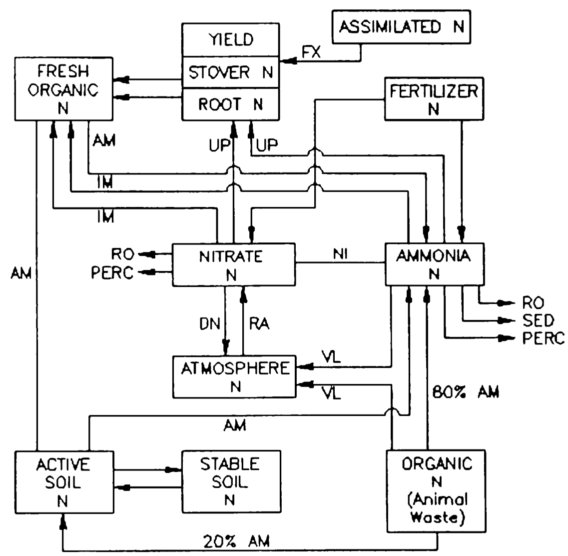

Figure 4: Schematic Representation of the GLEAMS Model Nitrogen Cycling Component

Management alternatives that affect N and P fate include dates and amounts of fertilization, fertigation, organic (animal waste) and inorganic (commercial) fertilizers, and removal of crop residue (bale peanut hay, burn small grain residue, etc). Split fertilizer applications reduce the maximum concentration in the soil that may be subject to runoff or leaching. Animal waste incorporated into the soil resembles a "time release" function due to the mineralization processes. A high initial loading from animal waste may have less potential impact than the same amount of N and P in inorganic fertilizer due to relative availability.

Tillage and soil temperature functions are included in the nutrient component. Tillage mixes the various pools of nitrogen and phosphorus in the soil, and incorporates surface matter (crop residue, animal waste, etc.) into the near-surface soil computational layers. Mean daily air temperature is used as a base and adjusted for soil cover and water content, to estimate soil temperature by computational soil layer. Soil temperature in each layer is used to adjust nitro-

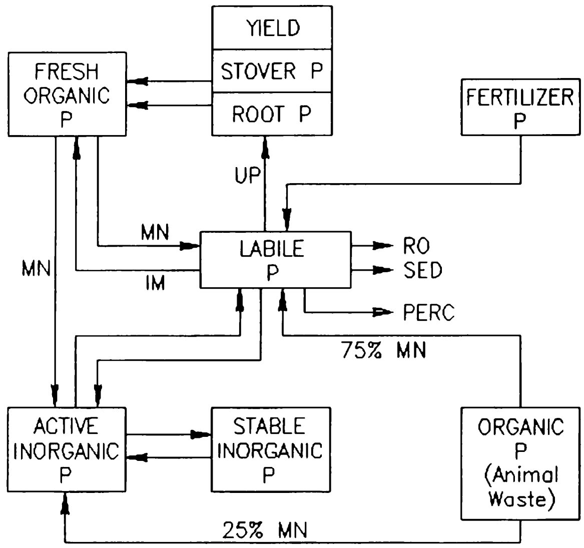

Figure 5: Schematic Representation of the GLEAMS Model Phosphorus Cycling Component

gen and phosphorus transformation rates. Soil temperature does not fluctuate as much as that of the air since the soil mass and soil water store more heat than the atmosphere and its moisture. A 5-day moving average is used to smooth that in the soil.

3 PROCESSES

Principal physical and chemical processes were identified in each component. The main processes in the pesticide and plant nutrient components are shown in figures 3-5. These were selected for emphasis in this paper.

3.1 Process Formulation

Processes in each component are formulated to interact as a function of time or condition. For example, soil evaporation, plant transpiration, pesticide degradation, and nutrient mineralization processes are simulated daily whether or not there is rainfall. If rainfall, irrigation, or snowmelt occur, other processes are actuated to simulate runoff, erosion, sediment transport, water, and chemical solute redistribution. Fertilization, pesticide application, and tillage are pulsed on dates specified by the user in the input file.

Leguminous plants such as alfalfa, clover, peanuts, soybeans, etc., assimilate (fix) nitrogen from the atmosphere. If soil nitrate and ammonium content are greater than about 5 parts per million (ppm) concentration in the soil, legumes take up nitrogen from the soil. If concentrations are less than 5 ppm, legumes assimilate the amount of nitrogen to satisfy the crop's need. **GLEAMS** must maintain a daily status of available nitrogen to determine which processes are activated--uptake or fixation.

Ammonification, nitrification, and denitrification processes occur at optimum rates at $35\,^{\circ}$C and are inoperative at $0\,^{\circ}$. Soil microbial population increases with temperature to the optimum, then decreases as temperature increases above the optimum. Also, microbial activity is a function of the soil water content. Ammonification and nitrification rates increase with soil water from zero at wilting point (1500 kPa matric potential) to a maximum at field capacity (33 kPa matric potential). Ammonification is assumed to cease at field capacity, and nitrification decreases to zero at saturation of the soil. Denitrification begins at field capacity and increases to a maximum rate at saturation. Thus, temperature and soil water content in each soil layer must be estimated each day to determine which processes are operative and to what degree. When a high water table occurs within the root zone, ammonification and nitrification can occur in the upper layers and denitrification can occur in the lower layers.

The carbon:nitrogen (C:N) ratio of crop residue is a factor in ammonification, also. If the C:N ratio is greater than 25, the ammonification process is reduced and immobilization (flow) of nitrate and ammonia to the crop residue occurs. The same process is active in the phosphorus cycle (figure 5), but the approximate C:P ratio is 200. Either process may control, and the net result may be immobilization instead of ammonification. Fresh organic carbon in crop residue and animal waste mineralize at different rates because of the relative C:N and C:P ratios (much lower in animal waste). C:N for wheat straw may be about 80 while that for soybeans may be about 24. C:N ratios of animal waste range from about 7 to 15 and C:P ratios range from about 40 to 75. C:N ratios for sawdust and pine straw may be as high as 200-300. Thus, ammonification and immobilization may be dominated by residue composition.

Nitrate moves entirely with water and is not adsorbed onto soil particles. Ammonium and phosphorus are partially adsorbed to clay particles, and are partitioned between the soil and water phases similar to pesticides. Thus, ammonium and phosphorus concentrations must be calculated in the water fraction of each soil layer on each day to calculate movement by evaporation, transpiration, infiltration, and percolation just as in the pesticide component.

Mass balance of nitrogen and phosphorus components are calculated and maintained on an annual basis. Harvestable crop yield, which includes grain and stover for corn silage, small grain and baled straw, multiple cuttings of hay, etc., is taken out of the system at harvest of each crop. The respective nitrogen and phosphorus content of the yield portion of the crop are taken out of the system in calculating the nutrient balance.

3.2 Process Computations

Daily process computations were estimated for each component of **GLEAMS.** An average of one hundred days of rainfall per year was assumed to produce 10 runoff and erosion events. The maximum 12 computational soil layers were assumed. The hydrology component is estimated to contain over 10,000 computations per year. The erosion component was estimated to include up to 20,000 computations. Over 200,000 annual computations were estimated for the maximum 10 simultaneous pesticide simulations. More than 150,000 computations were estimated for the plant nutrient component. The total for all components was estimated to be over 380,000 computations per year. Selection of the lowest level of output for each component results in about 30 seconds of model run time per year of simulation on a 386-16MHz personal computer with a math coprocessor operating with DOS.

4 SUMMARY

The **GLEAMS** model was developed to assess edge-of-field and bottom-of-root zone pollutant loads of sediment, pesticides, and plant nutrients from alternative agricultural and forestry management systems. The model is an assembly of complex interacting physical and chemical processes. It uses a daily time step in all components and processes, and it is computationally efficient. The model simulates impact of management on response of field-size areas to climatic input.

Over 380,000 computations are processed each year of simulation. Water and chemical balances are maintained on an annual basis.

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AUTHOR BIOGRAPHIES

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