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A Model of Carbon and Nitrogen Dynamics for Temperate Grasslands and Forests

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Abstract

In the last two decades, the importance of hydrological processes for ecosystem dynamics and the effects of plants on hydrological processes has become increasingly apparent. A better understanding of the relationship between plant growth (carbon and nitrogen distribution) and the hydrological characteristics of a catchment would improve ecological assessments and management of forests and grasslands.

TOPDNDC, developed for this study, is a detailed, semi-distributed, quantitative, ecohydrological model for predicting carbon and nitrogen dynamics in small temperate catchments. TOPDNDC establishes an explicit linkage between the biogeochemical process and the hydrology of catchments using the well-known and tested biogeochemical model DNDC and hydrological model TOPMODEL. The new model's ability to predict is assessed against field data.

The TOPDNDC computer model does not require use of high performance computers or large and expensive datasets, but it allows investigation in detail of how the locations and spatial patterns of biogeochemical processes shift across watershed topography in response to antecedent conditions and multiple temporal scales.

Application of the model to annual biomass production from a grassland shows very good agreement with the field data. The temperate forest simulation showed lesser agreement with field data collected along a transect in a watershed, but was able to reproduce the same patterns found in the field and with high correlations.

The difference in the results between the grassland and forest simulations may result, in part, from the intentionally simple link between the lateral and vertical water distribution components of the model.

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Chapter 1

Introduction

1.1 Human Alteration of Ecosystems

Technological developments have allowed the reduction of harmful social and economic consequences of imbalances between the supply and demand for ecosystem goods and services [*Daily, 1997*]. Nevertheless, humankind is still intimately connected to the natural environment, and the magnitude of human impacts on ecosystems, combined with growing human population and consumption, means that the challenge of meeting human demands will only grow.

The growing demand for ecosystem goods and services can no longer be met by tapping unexploited resources and trade-offs have become the rule [*Ayensu et al., 1999*]. Food supply can be increased by converting forests to agriculture, but that decreases the supply of goods of equal or greater importance such as clean water, timber, biodiversity, or flood control.

At the same time that humans are depleting the earth resources, the existing ecosystems are being impacted by refuse from human activities. Examples of direct effects on ecosystems abound [see *Goudie, 1993*]. However, other impacts are not so obvious, such as nitrogen deposition in forest and grasslands from reactive nitrogen species created by combustion (i.e. air pollution) and then transported by prevailing winds [*Aber et al., 1989*]. Terrestrial ecosystems are being over-fertilized to the point

of saturation since the increase in nitrogen sources are exceeding the biotic demand for this element [*Ågren and Bosatta, 1988; Aber, 1992; Stoddard, 1994; Peterjohn et al., 1996; Vitousek et al., 1997; Aber et al., 1998; Garten, 2000*].

In addition, the use of fossil fuels for energy, along with deforestation, is altering the global carbon cycle. Carbon dioxide in the atmosphere is increasing and is expected by many scientists to create significant global warming over the next several centuries.

The carbon and nitrogen cycles are intimately linked because both are the result of organismal activity that cycles these elements between the biosphere and the atmosphere.

Research is needed to improve our understanding of the interaction of carbon and nitrogen dynamics in watersheds. A better understanding of the relationship between carbon and nitrogen distribution and the hydrological characteristics of a catchment would improve ecological assessments and management of forests and grasslands. Also, better forecasting tools are needed to enable ecosystem management, such as managing land cover to support biodiversity, watershed protection, nitrogen retention, and carbon sequestration simultaneously.

1.2 Importance of Nitrogen

Nitrogen is an important element in the complex biogeochemical syntheses that are part of plant growth. In agriculture, many of the impressive improvements in plant productivity are attributed to increased applications of nitrogenous fertilizer to the soil.

Nitrogen is an essential element for all life. It represents roughly half of the minerals in a plant, and is a limiting factor for terrestrial primary productivity in most of the production areas of the world [*Gutschick, 1981*]. Nitrogen is unique

among soil resources that limit biological activity in that its primary source is the biological process of nitrogen fixation from the atmosphere.

Nitrogen availability is low in most natural ecosystems, and anthropogenically driven increases in nitrogen are having a major impact in aquatic and terrestrial ecosystems around the world [*Galloway et al.*, 1995; *Vitousek et al.*, 1997]. Excess nitrogen finds its way into surface and groundwaters when it leaches out of the soil and can be a serious health problem, in addition to its negative ecological effects.

1.3 Linkages of Carbon and Nitrogen

The roles of carbon and nitrogen are central in the functioning of all plants and tightly linked. The incorporation of nitrogen requires energy and a molecular framework supplied by carbon metabolism. In turn, the increase in biomass is often limited by available nitrogen. The production of new plant tissue requires nitrogen.

Carbon is acquired by leaves while nitrogen is almost exclusively acquired by roots. For growth to occur a proper balance between the functioning of the two organs (leaves and roots) must be maintained, especially because the chemical composition of a plant can only vary within narrow limits.

1.4 Dynamics of Hydrology, Carbon, and Nitrogen

Nitrogen in surface and groundwaters is influenced by hydrological compartment residence times and prevailing flowpaths in a given catchment. Current hydrological concepts link these flowpaths to terrain features, which can be quantified and scaled up through digital terrain models and geographic information systems. Carbon, nitrogen, and water are inextricably linked through the hydrological dynamics of landscapes. The capability to predict the spatiotemporal interactions of carbon, nitrogen, and water in terrestrial landscapes would be a major advance in the understanding and managing both water quality and ecosystem productivity.

Soil carbon, nitrogen, and water are critical limiting factors for plant growth in agriculture, forestry, and natural ecosystems. The interaction of limiting resources produces much of the variability in essential ecosystem processes such as net primary productivity (NPP).

1.5 Modeling

Every science involves theory, and every theory can be represented by a model of how the object of study works [Botkin, 1993]. We think and explain science through models of reality. A model is an intentional simplification of reality, simplified so that phenomena of interest can be examined, analyzed, and understood. While a model is necessary in science, it is also true that any model involves specific assumptions about how the world works. Thus the choice of a model is extremely important in the development of theory and of explanations.

Computer modeling is the best, and perhaps only, method for estimating plant growth for broad spatial (larger than small plots) and temporal scales [Barbour *et al.*, 1999]. Models estimate plant productivity either through regression equations of system variables or process-based algorithms. Numerous plant productivity or carbon models have been developed to study ecosystem responses under different conditions and at different scales, including Century, TEM, and Rothamsted [Jenkinson and Rayner, 1977; Parton *et al.*, 1988; Ågren *et al.*, 1991; Rastetter *et al.*, 1991; Smith *et al.*, 1997].

Research groups in the United States, Europe, and Australia have developed different models that combine ecological concepts of carbon and water distribution in a watershed. In some of these models, like RHESSys [Band *et al.*, 1993] and TOPOG-IRM [Hatton *et al.*, 1992], the ecological model is based on biogeochemical processes (ecosystem function) that estimate vegetation productivity by simulating the carbon and nitrogen cycles. In other models [O’Callaghan, 1996], the ecological

model is based on biogeography formulations (ecosystem dynamics) that determine vegetation distribution as a function of climate.

There have been several approaches to modeling the nitrogen dynamics in a watershed, but they have mostly involved simple models of nitrogen cycling and application at scales larger than hillslopes [e.g. *Creed et al.*, 1996; *Birkinshaw and Ewen*, 2000a].

1.6 Objective of the Study

The overall objective of this study is to develop a useful, quantitative, and appropriately scaled computer model of the spatial and temporal dynamics of carbon and nitrogen in small catchments ($<10 \text{ km}^2$) in grasslands and temperate forests. An appropriate computer model should not require the use of high-end computers or large and expensive datasets, but it should allow the investigation in detail of how the locations and spatial patterns of biogeochemical processes shift across watershed topography in response to antecedent conditions on multiple temporal scales.

The model establishes an explicit linkage between the biogeochemical processes and the hydrology of catchments, and the accuracy of its predictions can be assessed using available biogeochemical and hydrological data from field studies.

To successfully accomplish the overall objective of the study, the modeling effort was subdivided into three main tasks or sub-objectives:

- Improve an existing biogeochemical lumped parameter model to simulate biomass productivity and nutrient fluxes observed in field data collected in a grassland.
- Link water, carbon, and nitrogen dynamics and their availability in terrestrial ecosystems through the use of a deterministic, semi-distributed parameter hydrological model.

- Model the carbon and nitrogen dynamics of a forested watershed with the model developed above and compare the results against field data.

1.7 Limits of the Study

The results of this study include a calibrated ecohydrological computer model for temperate grasslands and forested catchments and a comparison of the biomass production in a grassland and the distribution of carbon and nitrogen in a forested watershed.

The research presented here focuses on hydrological and nutrient processes occurring at the hillslope scale. A larger scale would not allow the level of resolution necessary to discern nutrient dynamics occurring as a function of the hydrology of the area. Furthermore, modeling at the hillslope scale is critical for understanding physical processes governing surface and subsurface runoff generation and non-point source solute and particulate loading in complex terrains [*Gupta et al., 2000*].

This study does not explore hydrological and nutrient dynamics for large temporal scales like those required in climate change scenarios. Other ecohydrological models [*Creed et al., 1996*] and global carbon models [*Potter et al., 1993; Foley et al., 1996; Field et al., 1998; Lu et al., 2001*] have been used for those kind of studies. Both of these types of models are data intensive and require high-end computers to process large amounts of data coming from remote sensing satellites.

The model developed in this study does not address vegetation dynamics on the catchment, like forest succession or distribution of different vegetation types in the catchment, but allows vegetation properties as input data.

Chapter 2

Literature Review

2.1 Ecohydrological Models

2.1.1 Introduction

In the last two decades, the importance of hydrological processes in ecosystems dynamics and the effects of plants on hydrological processes have become increasingly apparent. Ecohydrology, an emerging discipline that involves hydrology and ecology, studies how individual plants or assemblages of plants are affected by and, in turn, influence hydrological processes [*Baird and Wilby, 1999*]. It is important to differentiate ecohydrology from hydroecology, the latter describes the study of ecological and hydrological processes in rivers and floodplains, the former, ecohydrology, relates to those same processes but on terrestrial ecosystems [*Baird and Wilby, 1999*].

The creation and use of ecohydrological models has improved the conceptual understanding of the interrelationship between hydrology and ecology, and also help formalize it. Ecohydrological models simulate the spatial patterns of ecological and hydrological storages and fluxes through the combined use of biogeochemical and hydrological models.

Two distinct types of ecohydrological models have been developed, regional and global models. Regional ecohydrological models generally apply to scales from

hillslopes to river basins. Their development has had two objectives, first to help manage our natural resources in view of the increasing pollution problems, and second to help investigate the relationship between ecology and hydrology in a scale amenable to testing and calibration of models.

Global models are more appropriately called global carbon models or biosphere models. They are being developed in an attempt to understand global biospheric processes and their potential response to human activity. Global models apply to large scales (whole earth), and therefore lack a sophisticated hydrological routing component if results are to be downscaled for regional use. See *Cramer et al. [2001]* for a review of several of these models. For completeness, a short description of two typical biosphere models, IBIS and RAMS-Century, is presented here.

2.1.2 Global Models

The Integrated Biosphere Simulator (IBIS) [*Foley et al., 1996; Kucharik et al., 2000*], is a comprehensive model of the terrestrial biosphere, representing a wide range of processes, including land surface physics, canopy physiology, plant phenology, vegetation dynamics and competition, and carbon and nutrient cycling. These processes are organized in a hierarchical framework and operate at different time steps, ranging from one hour to one year. Such an approach allows for explicit coupling of processes occurring on different time scales. IBIS generates global simulations of the surface water balance, the terrestrial carbon balance, and vegetation structure. It is designed to be incorporated directly within atmospheric general circulation models.

RAMS-Century [*Lu et al., 2001*], is a coupled Regional Atmospheric Modeling System (RAMS) and ecosystem (CENTURY) (see Section 2.2.2) modeling system developed to study global-scale two-way interactions between the atmosphere and biosphere. Both atmospheric forcings and ecological parameters are predicted

variables in the linked system. The atmospheric and ecosystem models exchange information on a weekly time step. CENTURY receives as input air temperature, precipitation, radiation, wind speed, and relative humidity simulated by RAMS. From CENTURY-produced outputs, leaf area index, and vegetation transmissivity are computed and returned to RAMS. In this way, vegetation responses to weekly and seasonal atmospheric changes are simulated and fed back to the atmospheric land surface hydrology model in RAMS.

2.1.3 Regional Models

A small number of research groups in the United States, Europe, and Australia have developed regional ecohydrological models, although some have been wrongly named hydroecological models instead.

In Europe, the two groups developing ecohydrological models have used them mainly to analyze the transport of nitrate in catchments [*Styczen and Storm, 1993; Birkinshaw and Ewen, 2000a*], and both have based the hydrological component of their model on the Système Hydrologique Européen (SHE) [*Abbott et al., 1986a*] (see Section 2.3.2). The model from England is called NITS/SHETRAN and the one from Denmark DAISY/MIKE-SHE.

NITS/SHETRAN [*Birkinshaw and Ewen, 2000b*] is an ecohydrological model created at the University of Newcastle in England consisting of two fully integrated, physically-based models for flow and transport in a catchment. One important aspect of this model set is that its components were developed specifically to be fully compatible with each other [*Birkinshaw and Ewen, 2000b*].

The Nitrate Integrated TranSformation (NITS) model simulates the state of soil carbon and nitrogen at a single point in space through the use of eight different pools. The pools represent mass balances for soil carbon and nitrogen decomposing at

three different rates, plus pools for ammonium and nitrate to calculate mineralization and immobilization rates.

SHETRAN, which is based on SHE (see Section 2.3.2), is a three-dimensional coupled surface and subsurface physically based and spatially distributed finite difference model for coupled water flow, multifraction sediment transport, and multiple, reactive solute transport in river basins [Ewen *et al.*, 2000]. Together, these two components are capable of simulating the concentration of nitrogen species and carbon in the soil, along with water flow and nitrate transport at every time step and location in a catchment. So far, NITS/SHETRAN has been used to model nitrogen fertilizer applications and the resulting nitrate leaching and the subsurface transport to the ground surface, then transport overland and through a river network [Birkinshaw and Ewen, 2000a]. NITS/SHETRAN is a complex and data intensive model. Its authors state that a preliminary data set may take at least a few weeks to prepare, require the use of a high-performance UNIX workstation, and take more than two hours of processing time per year of simulation [Ewen *et al.*, 2000]. NITS/SHETRAN lacks a plant growth component. Therefore, it is not possible to estimate plant biomass and biomass partitioning.

The other European model, DAISY/MIKE-SHE [Styczen and Storm, 1993], was created at the Danish Hydraulic Institute by combining two separate models, the DAISY model and the MIKE-SHE modeling system. This combined ecohydrological model allows the comprehensive three-dimensional modeling of nitrogen transformations and transport in catchments, from its application to the fields to the appearance as nitrate in surface water.

DAISY, its ecological component, is a one-dimensional soil organic matter model that simulates crop production, soil water dynamics and nitrogen dynamics under various agricultural management practices [Hansen *et al.*, 1991a; Mueller *et al.*, 1996]. DAISY is an advanced and complex agro-ecosystem model. However, it

is currently parameterized only for the wet temperate climate of North-Western Europe, modifications to the crop modules may be necessary for other locations [Mueller *et al.*, 1996]. A more detailed description of DAISY is presented in Section 2.2.2.

MIKE-SHE, a further development of the SHE model (see Section 2.3.2), is a comprehensive deterministic, distributed and physically-based modeling system for the simulation of all major hydrological processes occurring in the land phase of the hydrological cycle [Refsgaard and Storm, 1995; Storm and Refsgaard, 1996]. MIKE-SHE has a modular structure that allows add-on components, with DAISY being one of these components. The reason for combining DAISY and MIKE-SHE, besides its parallel development in Denmark, was that DAISY is under many conditions compatible with MIKE-SHE in the unsaturated flow description [Styczen and Storm, 1993]. Therefore, the two models are run sequentially, with DAISY first producing calculations of water and nitrogen behavior from the soil surface and through the root zone, and the result of this percolation of water and nitrate at the bottom of the root zone is then used as input to MIKE-SHE calculations for the remaining part of the catchment [Refsgaard *et al.*, 1999]. Recently, the two models were integrated, so the chemical reactions and temperature calculations take place in DAISY while the flow and solute transfer take place in MIKE-SHE [Styczen *et al.*, 1999]. MIKE-SHE and the DAISY add-on are commercially available for PC computers with the Windows operating system. As such, they are finished products and expensive, with no access to the source code for modifications.

The ecohydrological models developed in Europe seem to originate from the need to further understand and predict non-point pollution from agricultural areas, in response to increased use of animal manure and fertilizer. During the last decades, countries in Europe have had to deal with an increased nitrate load in their groundwater, streams, lakes, and coastal areas.

The ecohydrological model TOPOG_IRM was developed by researchers at the Commonwealth Sciences and Industrial Research Organisation (CSIRO) Division of Water Resources in Australia. TOPOG_IRM [*Hatton et al., 1995; Dawes et al., 1997; Zhang et al., 1999*] is a pseudo three-dimensional biophysically based distributed parameter model that predicts the dynamic interactions within the soil-vegetation-atmosphere system over a catchment. The model consists of three sub-models that simulate energy, water, and carbon (plant growth) balances [*Dawes et al., 1997*]. TOPOG_IRM predicts daily rainfall interception, vertical and horizontal soil water distribution, the horizontal distribution of daily evapotranspiration from both the overstory and understory vegetation, daily evaporation from the soil-litter layer, and daily streamflow. It also predicts daily changes in leaf, stem and root carbon of both the understory and overstory, and leaf fall and decomposition [*Vertessy et al., 1996*].

The Integrated Rate Methodology (IRM), the ecological component of TOPOG_IRM, is a multifactor plant growth model based on a plant growth index to estimate the effective relative growth rate from a potential relative growth rate [*Wu et al., 1994*]. This methodology is a generalization of Michaelis-Menten kinetics to multiple substrates [*Wu et al., 1994*]. The growth index simultaneously integrates the relative effects of light, nitrogen, water, and CO₂ as modified by temperature and vapor pressure deficit on the modeling of carbon assimilation [*Hatton et al., 1995*]. Maintenance respiration is calculated as a function of temperature, and net photosynthesis is computed as assimilation less total respiration. Growth respiration is assumed to be a constant fraction of allocated carbon. The balance between carbon assimilation and respiration and the allocation of carbon is handled through the use of five carbon pools (litter, leaf, root, live stem, and a soluble pool expressed as a fraction of leaf carbon)[*Vertessy et al., 1996*]. The litter pool decays as a function of temperature and water.

TOPOG [O’Loughlin, 1990] is a deterministic, distributed-parameter, hydrological modeling package developed in Australia. It consists of over thirty FORTRAN and C programs designed for a variety of hydrological problems [Vertessy *et al.*, 1993]. A set of these programs are terrain analysis routines that constitute the “kernel” of TOPOG and are used to generate a network of catchment elements in which water balance computations are made. The rest are application modules used when needed for diverse scenarios like forest water yield, absorption trenches, erosion, etc. Non-topographic spatial attributes, such as soil and vegetation properties are accounted for in TOPOG via overlay routines similar to those found in geographic information systems (GIS) [Vertessy *et al.*, 1993]. For a detailed description of TOPOG see Section 2.3.2.

TOPOG_IRM concentrates only on the hydrological aspects of plant growth, the model does not account for reproductive material of plants, neither does it perform nutrient leaching and cycling (availability of nutrients is a spatially explicit constant)[Dawes *et al.*, 1997].

In the United States, several models that relate the ecology of an area with its hydrology have been developed. However, only RHESSys can be considered a regional ecohydrological model. The other models were developed for global scale applications (see Section 2.1.2).

The Regional Hydroecological Simulation System (RHESSys) (<http://www.unc.edu/depts/geog/them/index.html>) [Band *et al.*, 1991; Band, 1993; Band *et al.*, 1993] is an ecohydrological model developed as a collaborative effort between research groups at the University of Toronto (now at the University of North Carolina at Chapel Hill), the University of Montana, and the National Aeronautics and Space Administration (NASA)/Ames Research Center. RHESSys combines distributed water flow modeling with an ecophysiological canopy model based on BIOME-BGC and a climate interpolation scheme based on MT-Clim. Previous versions of RHESSys

used FOREST-BGC as their ecological model. RHESSys has been applied to hydrological investigations, forest productivity, regional scale water and carbon budgets, climate change scenarios, and nitrogen leaching [*Band et al.*, 1996; *Creed et al.*, 1996; *Baron et al.*, 1998; *Creed and Band*, 1998; *Band et al.*, 2001].

The ecological component of RHESSys, BIOME-BGC (see Section 2.2.2), generalizes the coniferous forest logic in FOREST-BGC to other biomes and implements a more general ecosystem process framework [*Running and Hunt*, 1993]. The model uses a mechanistic approach to canopy interception and evaporation, transpiration, photosynthesis, growth and maintenance respiration, dynamic carbon allocation above and below-ground, litterfall, decomposition and nitrogen mineralization [*Running and Coughlan*, 1988; *Running and Gower*, 1991]. BIOME-BGC is particularly sensitive to leaf area index (LAI) for defining the vegetation canopy and climate for controlling the processes [*Running and Hunt*, 1993].

The MounTain Microclimate Simulator (MT-Clim) is a micrometeorology model [*Running et al.*, 1987] that uses topography and user-supplied base station information to derive spatially variable climate variables such as radiation and to extrapolate input climate variables over topographically varying terrain.

Originally, RHESSys utilized TOPMODEL (see Section 2.3.3) to model soil moisture redistribution and runoff production in a watershed. It now includes two approaches. The first approach is still TOPMODEL [*Beven and Kirkby*, 1979], which is a semi-distributed model that distributes hillslope soil moisture based on a distribution of a topographically defined wetness index. The second approach is an explicit routing model adapted from DHSVM (see Section 2.3.2) that models saturated subsurface throughflow and overland flow via explicit connectivity. An important modification from the grid-based routing in DHSVM is the ability to route water between arbitrarily shaped surface elements. This allows greater flexibility in

defining surface patches and varying shape and density of surface tessellation [*Band et al.*, 2001; *Tague and Band*, 2001].

Table 1 presents a qualitative comparison of the operational parameters for the regional ecohydrological models described in this chapter. Currently, there is no available low-cost, easy-to-use ecohydrological model.

2.2 Biogeochemical Models

2.2.1 Introduction

Biogeochemistry and biogeography models are two general classes of ecosystem models for studying the impacts of environmental change and management practices on ecosystems [*Neilson and Running*, 1996]. This review describes biogeochemical models since the interest is in estimating vegetation productivity by simulating carbon and nitrogen cycles (see Section 1.5).

Biogeochemical models, some of which are also called soil organic matter (SOM) models, determine how well vegetation can grow and persist, given the knowledge of what lives there. These models are able to determine vegetation growth by simulating the processes of carbon assimilation, autotrophic and heterotrophic respiration and decomposition based on inputs of radiation, temperature, precipitation, and nutrient availability.

Table 1: Comparison of regional ecohydrological models.

Model	Data Needs	Ease of Use	Hardware Needs	Type of Use
NITS/SHETRAN	high	low	high	research
DAISY/MIKE-SHE	high	medium	medium	commercial
TOPOG_IRM	medium	low	high	research
RHESSys	high	medium	high	research

Biogeochemical models first appeared in the literature in the 1940's when *Jenny* [1941] used a first-order decay equation to describe the accumulation or loss of carbon from soils. The large number of biogeochemical models published since then make it important to develop ways to compare and organize information about these models, particularly with respect to global models, where the intercomparison of global NPP models provides an effective tool to check model consistency, given that neither absolute measures nor direct model validations of global terrestrial NPP are feasible [e.g. *Cramer et al.*, 1999].

Until recently, there was not much interest in comparing different ecosystem models, and most models were developed without using components from existing models [*Parton*, 1996]. However, since the beginning of the 1990's, there has been interest and funding to compare ecosystems models to try to determine if new models are needed and also due to their increased use in the evaluation and solution of environmental problems [*VEMAP Members*, 1995; *Cramer et al.*, 1999, 2001].

Classification of SOM models has varied, some researchers classify the models according to the number of decomposition compartments: none, one, two, and multiple compartments [*Jenkinson*, 1990]. Others have organized the SOM models with respect to energy and matter into either organism-oriented models or process-oriented models, or with respect to the type of environmental conditions they require to operate, temporal or spatial scales that are applicable, the use of soil layering, etc. [*McGill*, 1996]

Several reviews of biogeochemical models have appeared in the literature. *Smith et al.* [1997] evaluated nine different SOM models using seven long-term data sets and determined that no one model performed better than all others. *Ågren et al.* [1991] reviewed several biogeochemical models for conifer and grassland ecosystems to determine their applicability in the prediction of the impact of a future climate change arising from increased atmospheric carbon dioxide concentration. *Hanson*

et al. [1985] compared the methodology used by nine grassland models to simulate plant production. Several reports by the Vegetation and Ecosystem Modeling and Analysis Project (VEMAP) [*VEMAP Members*, 1995; *Schimel et al.*, 1997; *Pan et al.*, 1998] compare the simulations of three biogeochemical models to climate change and CO₂ doubling at the continental-scale. *Cramer et al.* [1999] compared seventeen global terrestrial biogeochemical models with respect to annual and seasonal fluxes of net primary productivity (NPP) for the land biosphere.

2.2.2 Existing soil organic matter models

The Rothamsted model, also called the RothC model [*Jenkinson and Rayner*, 1977; *Jenkinson*, 1990; *Coleman and Jenkinson*, 1996], is the first widely used biogeochemical model and one of the simplest. The model is based on the work performed in the long-term field experiments on Rothamsted, England. RothC simulates topsoil processes only since it does not contain a submodel for plant production, but its data input requirements are few and easily obtainable. RothC uses four active compartments and a small amount of inert organic matter to determine the decomposition processes occurring in the soil. The four active compartments are decomposable plant material, resistant plant material, microbial biomass, and humified organic matter. Each of these four compartments decompose by a first-order process with its own characteristic rate determined by data from long-term field experiments. As such, this models works best in situations similar to those for which it was originally parameterized (i.e. arable soils in the temperate zone). Nitrogen and carbon dynamics are not interconnected. The model uses a monthly step for output calculations on a years-to-century time scale.

The Century model (<http://nrel.colostate.edu/projects/century/>) [*Parton et al.*, 1987, 1988, 1994], currently bears little resemblance to the Rothamsted model. However, earlier versions of the Century model were based on the Rothamsted

model [*Parton et al.*, 1994]. Century simulates long-term (decades to centuries) soil organic matter dynamics, plant growth and cycling of N, P, and S. The model runs using a monthly time step, and the major input variables are monthly average maximum and minimum air temperature, monthly precipitation, lignin, N, P, and S content of plant material, soil texture, and atmospheric and soil N. Century separates litter into metabolic and structural forms, and soil organic matter into active, slow, and passive compartments [*Parton et al.*, 1987]. It includes a simplified water budget model that calculates evaporation and transpiration losses, water content of the soil layers, snow water content, and saturated water flow between soil layers. Century was originally developed for grasslands, but has since been extended to agricultural crops, forests, and savanna systems [*Smith et al.*, 1997]. It has been used to simulate carbon accumulation during soil formation, and changes in soil carbon storage following climate change scenarios [*Smith et al.*, 1997].

The biogeochemical model DAISY (<http://www.dina.kvl.dk/~daisy/>) was developed independently of other SOM models by a research group in Denmark in the early 1990's. However, the structure of its SOM submodel resembles that of Century and RothC, and it was calibrated with data from the Rothamsted long-term field experiment [*Jensen et al.*, 1997; *Mueller et al.*, 1998]. DAISY uses soil carbon pools and turnover rates to describe mechanistically the turnover of nitrogen in soil [*Jensen et al.*, 1997]. It simulates the fluxes of carbon and nitrogen in a one-dimensional soil-plant-atmosphere system, allowing for five different soil horizons and a number of soil layers divided on the basis of physical and chemical soil characteristics [*Hansen et al.*, 1991a,b; *Mueller et al.*, 1996]. DAISY consists of submodels for soil water movement (Richard's equation) including solute movement, soil temperature, soil organic matter dynamics, soil mineral nitrogen, crop growth, and farming system management (soil tillage, harvest, etc.). DAISY is not currently applicable to model forests because it does not incorporate modules for

tree growth, cannot simulate soil water and temperature dynamics in a forest system, does not include leaching of dissolved organic substances, or the effect of low pH on decomposition [Jensen *et al.*, 1997]. Recently, DAISY has been rewritten to facilitate interactions with other models [Abrahamsen and Hansen, 2000], and for potential use with remotely sensed data [van der Keur *et al.*, 2001].

The DeNitrification-DeComposition (DNDC) model [Li *et al.*, 1992a,b] is a process-oriented simulation model of soil carbon and nitrogen biogeochemistry. DNDC utilizes some concepts, formulas, and parameters from other models. The structure of soil organic matter pools follows that of the NCSOIL model by Molina *et al.* [1983], the denitrification sequence is taken from a closed system model from Leffelaar and Wessel [1988], and the hydraulic conductivity equations come from the models developed by Mualem [1986] and Clapp and Hornberger [1978]. Originally, DNDC consisted of three submodels (soil-climate, decomposition, and denitrification) and applied to agricultural soils only [Li *et al.*, 1992a]. Later versions of the model also include a plant growth submodel and cropping practice routines [Li *et al.*, 1994a], and applications to forest soils [Li *et al.*, 2000; Stange *et al.*, 2000]. A unique feature of DNDC is the hourly-to-daily time scale for calculating N₂O and NO emissions from soils. DNDC requires few input parameters and has been tested against field measurements in various croplands and forestlands across the world, either on soil organic matter or on trace gas emissions [Li *et al.*, 1992b, 1997]. It has also been used for studies on alternative agricultural practices in soil carbon sequestration and mitigation of greenhouse gases, and for estimation of regional trace gas emissions [Li *et al.*, 1994b].

The Biome BioGeochemical Cycles model (BIOME-BGC) (<http://www.forestry.umd.edu/ntsg/models/>) [Running and Hunt, 1993; VEMAP Members, 1995] is a multibiome generalization of FOREST-BGC [Running and Coughlan, 1988; Running and Gower, 1991], a model originally developed to simulate forest

stand development through key processes involved in the carbon, nitrogen, and water cycles. BIOME-BGC simulates interannual variability in net primary production and heterotrophic respiration on a global scale using a two time-step system. A daily time-step uses all-sided leaf area index for the simulation of photosynthesis, autotrophic and heterotrophic respiration, and the hydrological budget. The annual time-step handles the allocation of carbon and nitrogen, litterfall and turnover, and net nitrogen mineralization [Hunt *et al.*, 1996]. The input parameters consist of detailed daily weather data, and vegetation and soils conditions. BIOME-BGC is parameterized for seven structural vegetation biomes: deciduous needleleaf and broadleaf forests, evergreen needleleaf and broadleaf forests, shrubs or deserts, and C₃ and C₄ grasslands [Churkina and Running, 1998]. BIOME-BGC relies primarily on the hydrological cycle and water availability for controlling carbon uptake and storage [VEMAP Members, 1995; Pan *et al.*, 1998]. Changes in leaf nitrogen are prescribed, and nitrogen cycling plays no role in controlling nitrogen allocated to canopy biomass. BIOME-BGC focuses on transpiration and leaf area responses rather than on feedbacks from nutrient cycling. This allows BIOME-BGC to predict short-term decreases in NPP due to drought and the effects of moisture storage in the soil. However, it does not fully implement the effects of nitrogen availability to control assimilation responses to elevated CO₂ [Hunt *et al.*, 1996; Pan *et al.*, 1998]. BIOME-BGC as well as its predecessor, FOREST-BGC, have undergone extensive validation of the simulated water and carbon budgets in different North American ecosystems.

The Terrestrial Ecosystem Model (TEM) is a process based ecosystem simulation model specifically designed to estimate the spatial and temporal distribution of carbon and nitrogen at continental to global scales [Raich *et al.*, 1991; Rastetter *et al.*, 1991; McGuire *et al.*, 1992]. TEM uses spatially referenced information (grid-cell resolution: 0.5° latitude × 0.5° longitude —3,090 km² at the equator) on climate,

elevation, soils, and vegetation to make monthly estimates of the major carbon and nitrogen fluxes and pool sizes. The model is highly aggregated, that is, vegetation and soil are assumed to be distributed homogeneously within each grid cell. TEM consists of five pools (C in vegetation, N in vegetation, C in soil, organic N in soil, inorganic N in soil) and nine fluxes (gross primary productivity, plant respiration, C in litter production, soil respiration, N input to the ecosystem, N uptake by vegetation, N in litter production, net N mineralization, N lost from the ecosystem). A newer version of TEM splits the N in vegetation into structural and labile pools, with the corresponding increase in fluxes (now 12 fluxes) [McGuire *et al.*, 1995]. Hydrological inputs for TEM are determined by a separate water balance model that uses the same climatic data and soil specific parameters as used in TEM [Melillo *et al.*, 1993]. Some of the vegetation specific parameters in TEM can be defined from published information, other must be determined by calibrating the model to the steady state fluxes and pool sizes of an intensively studied field site. TEM has been used primarily for estimation of net primary productivity and carbon storage under climate change scenarios at a global scale.

There are several other biogeochemical models, such as CANDY, LINKAGES, and NCSOIL. They have similarities and differences from the previously described and more widely-used models. In general, these other models describe soil organic matter processes as pools of carbon and nutrients with different decomposition rates, though some of them (e.g. LINKAGES) use a system of cohorts instead.

There are several other models of global biogeochemistry [see Schimel *et al.*, 1997; Pan *et al.*, 1998; Cramer *et al.*, 1999]. However, representations of biogeochemical processes at large scales may not be appropriate for regional or hillslope scale applications, and the downscaling of the processes may not represent realistic situations.

2.3 Hydrological Models

2.3.1 Introduction

There are different approaches for modeling the hydrological behavior of a watershed. These approaches are generally classified according to how they address different issues, such as process description, scale, and technique of solution [Singh, 1995]. At the broadest level, the major issue is the spatial scale of the hydrological processes taking place in the watershed. Different hydrological questions arise at various spatial scales. Gupta *et al.* [2000] defines these scales as global scale, continental scale, medium to large drainage basin and aquifer scale, and hillslope scale. The appropriate model is one that represents the relevant processes occurring at the scale of interest or fits the purpose of study.

Usually, different models are created for applications at different scales. A simple water budget model may be appropriate at the global scale for use in global circulation models, but will be overly simple for processes occurring in a hillslope. This scale approach does not preclude applying a model to a scale different from that for which it was developed. Nevertheless, the relevant processes on the new scale may be other than the ones modeled, unless the processes can be made scale invariant. In fact, scale dependence and scale invariance are currently active areas of research in hydrology [Sposito, 1998].

In this study, the interest is on hydrological processes occurring at the hillslope scale. A larger scale would not allow the level of resolution necessary to discern nutrient dynamics occurring due to the hydrology of the area. Modeling at this scale is critical for understanding physical processes governing surface and subsurface runoff generation, and non-point source solute and particulate loading in complex terrains.

Furthermore, the interest in the spatial variability of hydrological processes occurring within the catchment precludes the use of lumped models. Lumped models assume that hydrological processes occur uniformly over the entire catchment, and that all areas behave in the same manner. Lumped models are well suited for the simulation of the rainfall-runoff process when there is a long enough hydrological record to calibrate the model, and the results are needed in only a few points in the catchment. Unlike distributed models, they are unable to provide information on changing hydrological conditions in the different parts of the catchment. They rarely discriminate between the many intervening processes which occur between rainfall hitting the ground and runoff arriving at the stream. Figure 1, shows the typical structure of a lumped model. Other models that are hydrologically distributed, but lump land processes (no distributed soil moisture calculations) such as HEC-HMS, are not usable for the purpose of this study.

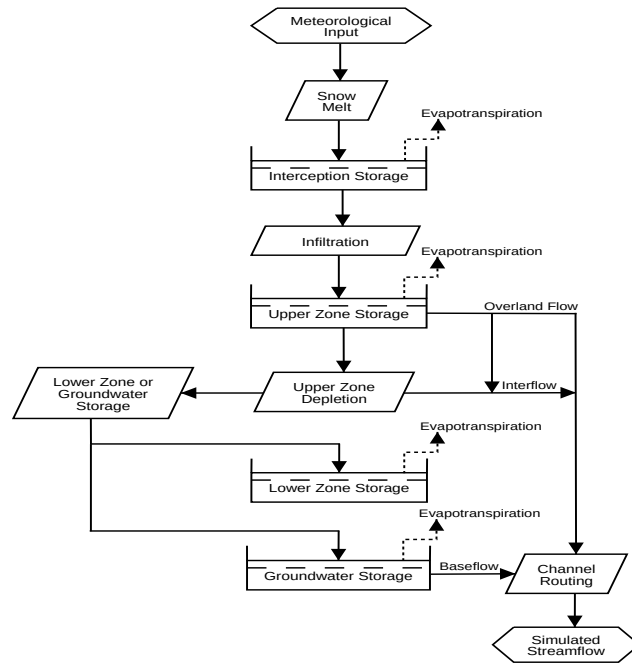


Figure 1: Structure of a hydrological lumped model [from *Refsgaard, 1996*].

Distributed models account explicitly for the spatial variability of processes and characteristics of a watershed. They give a detailed and potentially more correct description of the watershed than lumped models, but require the direct calculation of water and energy flows from the governing continuum equations, such as Saint Venant equations for overland and channel flow, Richard's equation for unsaturated zone flow, and Boussinesq's equation for groundwater flow. Figure 2, presents a conceptual diagram of a catchment in a distributed model.

Semi-distributed models try to model the dominant spatially-variant processes of hydrology rather than be overly detailed in all processes. They avoid the modeling of processes that are extremely difficult to prove or parameterize. Semi-distributed models account explicitly for the spatial variability and the direct use of spatial data such as topography and channel system, but lump calculations of some hydrological variables [Refsgaard, 1996]. They normally have the spatial variability of the soil properties built into the process equations.

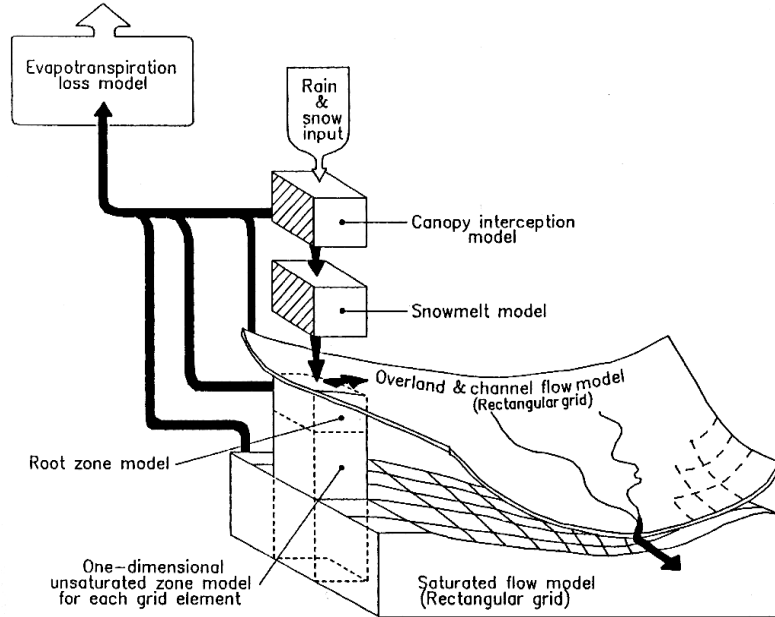


Figure 2: Diagram of a hydrological distributed model [from Bathurst et al., 1995].

There is a current debate among hillslope scale modelers, on whether physically based, fully distributed models, being more complex and parameterized, have a better accuracy of prediction than simpler, more robust, and more easily calibrated semi-distributed models [Beven, 1996]. Fully distributed models take into account spatial variations in all variables and parameters, and give a detailed description of the hydrological processes in the catchment [Refsgaard, 1996]. However, these models require large amounts of data, are computationally complex, and difficult to calibrate.

2.3.2 Fully distributed models

The Distributed Hydrology Soil Vegetation Model (DHSVM) (<http://maximus.ce.washington.edu/~nijssen/docs/DHSVM/>) developed by the University of Washington and the Battelle Memorial Institute [Wigmosta et al., 1994] is a fully distributed, physically based hydrological model that includes canopy interception, evaporation, transpiration, snow accumulation and melt, and runoff generation via the saturation excess mechanisms. DHSVM was created for use in complex terrains, such as mountainous regions, where surface characteristics (topography, vegetation, and soils) and meteorological conditions (precipitation, wind speed, solar radiation, and air temperature) vary strongly in space.

DHSVM uses digital elevation data (DEMs) to model topographic controls on incoming solar radiation, precipitation, air temperature, and downslope water movement. It provides a simultaneous solution to the energy and water balance equations for every grid cell in the watershed at each time step. Grid cells are hydrologically linked through a quasi three-dimensional saturated subsurface transport scheme, which redistributes the downslope soil moisture explicitly, that is pixel-by-pixel. Each grid cell in the DEM is assigned a surface cover, consisting of overstory and understory vegetation, and soil properties at three levels, upper rooting zone,

lower rooting zone, and saturated zone. Local meteorological conditions are prescribed for each grid cell at a specified distance above the overstory.

Evapotranspiration is modeled using a Penman-Monteith approach, where the overstory is allowed to remove water from both the upper and lower root zone, and the understory only takes water from the upper zone. Solar radiation and wind speed are attenuated through the two canopies based on cover density and leaf area index (LAI), providing separate values for the overstory, understory, and soil. Stomatal resistance is calculated for each story based on local air temperature, the vapor pressure deficit, soil moisture conditions, and the photosynthetically active radiation flux. Soil water evaporation is dependent on the climatic demand, modulated by the soil's ability to supply water.

Snow accumulation and melt is simulated using a single-layer energy balance model that explicitly incorporates the effects of topography and vegetation cover on the energy exchange at the snow surface. Unsaturated moisture movement through the two rooting zone soil layers is calculated using Darcy's law. Discharge from the lower rooting zone recharges the local (grid cell) water table. Each grid cell exchanges saturated zone water with its eight adjacent neighbors as a function of water table depth, soil characteristics, and local topography, resulting in a transient, quasi three-dimensional representation of saturated subsurface flow. Return flow and saturation overland flow are generated in locations where grid cells water tables intersect the ground surface.

DHSVM is one of the newest hydrological models and therefore has not been tested as extensively as the other models discussed here. A modification of DHSVM is used in RHESSyS (Section 2.1.3) for soil moisture redistribution through saturated throughflow and associated runoff production [*Tague and Band, 2001*].

The Système Hydrologique Européen (SHE) is a physically based, distributed parameter catchment modeling system created jointly by the Danish Hy-

draulic Institute, the British Institute of Hydrology and the French company SOGREAH [Abbott *et al.*, 1986a,b]. SHE integrates surface and subsurface representation of water movement through a river basin, incorporating the major elements of the land phase of the hydrological cycle, such as evapotranspiration and interception, overland and channel flow, unsaturated zone flow, saturated zone flow, snowmelt, and channel/surface aquifer exchange [Bathurst *et al.*, 1995].

The modular software design of SHE allows the addition of different components using only data exchanges to link the components. Each hydrological process is allocated its own component and the simultaneous operation of all the components is controlled by the central FRAME component [Abbott *et al.*, 1986b]. Dummy components can be used when one or more hydrological processes are irrelevant to a particular application. All the hydrological processes of water movement are modeled by finite difference representations of the partial differential equations of mass, momentum, and energy conservation, or by empirical equations derived from independent experimental research [Abbott *et al.*, 1986b].

The interception component calculates net rainfall reaching the ground through the canopy, the amount of water stored in the canopy, and the evaporation from the canopy. Interception is modeled as an accounting procedure for canopy storage. The evapotranspiration component calculates actual evapotranspiration based on the Penman-Monteith equation. It is computed as a loss term to use it in the calculation of soil moisture changes by the unsaturated zone component. Extraction of moisture for transpiration from the root zone is distributed according to the vertical distribution of root mass in the root zone. Moisture for the soil evaporation is drawn from the top of the soil column.

The overland and channel flow component uses topographic, channel shape and flow resistance parameters to route surface water. The depth of surface water available for runoff is determined from the net rainfall and evaporation rates supplied

by the interception and evapotranspiration components, and from the soil infiltration rate determined by the unsaturated zone component. There is also an exchange between channel and aquifer to allow for seepage losses and groundwater input. Both the overland flow and the channel flow are modeled by approximations of the Saint Venant equations of continuity and momentum.

The unsaturated zone flow component determines the soil moisture content and tension distributions above the water table. This component is modeled based on the one-dimensional Richards equation and solved by an implicit finite difference scheme. In the original SHE model, up to four soil layers with different characteristics could be incorporated in a simulation.

The saturated flow component determines the phreatic surface level and the flows, assumed to be horizontal only, in the saturated zone of an unconfined aquifer, stream/aquifer interactions, groundwater seepage at the ground surface, and artificial groundwater extraction. The saturated flow is modeled by the nonlinear Boussinesq's equation, assuming laminar flow in an anisotropic, heterogeneous aquifer.

The snowmelt component uses snowpack, vegetation parameters, and meteorological input data, to predict the transfer of moisture and the variation in snowpack thickness resulting from the processes of precipitation onto the snowpack, snowmelt from the snowpack, lateral spatial variations in snowpack conditions, and interception and evapotranspiration in the presence of a snowpack and at air temperatures below freezing. Energy and mass fluxes are both modeled within the snowpack.

SHE has been a starting point for the development of several other distributed hydrological models, such as MIKE-SHE (<http://www.dhisoftware.com/mikeshe/>) and SHETRAN (<http://www.ncl.ac.uk/wrgi/wrsrl/models.html>). These newer models are either further developments of the processes in SHE, or additions of newer components to the SHE core like sediment transport or solute

transport. The SHE “technology” has been used and tested in many places around the world.

TOPOG (<http://www.clw.csiro.au/topog/>) is a physically based, distributed parameter catchment modeling framework developed by a large group of scientists from the Commonwealth Scientific and Industrial Research Organisation (CSIRO) Land and Water and the Cooperative Research Centre for Catchment Hydrology (CRC CH) in Australia [*O’Loughlin, 1990; Vertessy et al., 1993; Dawes and Short, 1994; Hatton et al., 1995*]. It has its origin in the WETZONE program, developed by *O’Loughlin [1986]* to predict surface saturation zones by topographic analysis, but has undergone radical change since then.

TOPOG is composed of a “kernel” and several application modules. The kernel consists of a set of terrain analysis routines that are used to generate a network of catchment elements in which water balance computations are made. The terrain analysis procedures use vector elevation data of the area to be modeled, and apply a set of topological rules to define the catchment boundary, and segment the catchment into a network of interconnecting hillslope elements. The network of elements is arranged around critical topographic features such as peaks, saddles, ridges, drainage lines and stream confluences, which result in a series of adjacent hillslope elements that diverge or converge according to local terrain [*Dawes and Short, 1994*]. These terrain analysis procedures are similar to those in the TAPES-C package used by the distributed rainfall-runoff model THALES [*Grayson et al., 1995*].

The TOPOG kernel also calculates the key topographic quantities that influence how water moves in hilly terrain (e.g. slope, upslope contributing area). The network of elements created by TOPOG provides a computationally effective means of routing surface and subsurface flows in complex topography, since the flux equations need to be solved in a single downslope dimension only. However,

this imposes the limitation of no lateral flow diffusion between hillslope elements [Vertessy *et al.*, 1993].

On top of the kernel, several application modules designed for specific modeling problems can be run. These applications include IRM (see section 2.1.3) that solves water, energy and carbon balances, and TOPOG_Yield for modeling transient unsaturated—saturated flow. Regardless of the application, the hydrological components (soil water dynamics, evapotranspiration, etc.) are modeled similarly on a daily time step.

Infiltration of net rainfall and the vertical redistribution of water in the soil is accomplished through a finite difference numerical solution of the Richards equation for each hillslope element [Vertessy *et al.*, 1993]. The solution assumes isotropic soils and accounts for matrix flow alone. Following the development of a water table, water is moved laterally according to the saturated hydraulic conductivity and the local hydraulic head. Overland flow, whether resulting from infiltration excess or surface saturation, and leakage to the deep groundwater system are treated explicitly.

Daily transpiration and soil evaporation are calculated with base inputs of maximum and minimum daily air temperature, mean daily vapor pressure deficit, and total daily direct and diffuse solar radiation incident on the horizontal plane. Solar radiation is modulated across the catchment; direct radiation according to the slope and aspect of each hillslope element, diffuse radiation is modified by slope alone. Net longwave radiation is partitioned, according to the Beer-Lambert law, between the canopy and the ground surface based on canopy leaf area (LAI), albedo, and a specified light-extinction coefficient. Before partitioning, the energy required to evaporate canopy intercepted water is deducted from the net longwave radiation. Soil evaporation is computed by the method of Choudhury and Monteith [Vertessy *et al.*, 1993], based on the net longwave radiation received at the ground surface and the

hydraulic conductivity of the uppermost soil layers. Transpiration is calculated using the Penman-Monteith equation. Water is extracted from the soil profile according to the soil water potential and relative rooting density after transpiration is computed. Canopy interception is determined via a single storage term defined as a function of LAI. Each day, rainfall is prevented from reaching the ground until this storage is filled.

TOPOG has been used in different parts of the world for a variety of applications like waterlogging and dryland salinity, catchment water yield, stormflow runoff production, soil erosion and deposition, land disposal of treated effluent, forest establishment and harvesting, landslide hazard assessment, and ecologic habitat assessment. TOPOG consists of over thirty FORTRAN and C programs, some of them interactive, entailing the use of mouse-driven menus and high level graphics functions. The full TOPOG package will only run on UNIX workstations.

2.3.3 Semi-distributed Models

TOPMODEL (a TOPography based hydrological MODEL) (<http://www.es.lancs.ac.uk/hfdg/topmodel.html>) is the only widely available and tested semi-distributed model. It was developed by *Beven and Kirkby* [1979] in England based on the concept of the topographic index proposed by *Kirkby* [1975]. TOPMODEL is not a hydrological modeling package, but a set of conceptual tools that can be used to simulate hydrological processes in a relatively simple way [*Beven and Kirkby*, 1979; *Beven et al.*, 1995; *Beven*, 1997].

TOPMODEL reproduces the hydrological behavior of catchments in a semi-distributed way, in particular the dynamics of surface or subsurface contributing areas. It attempts to combine the computational and parametric efficiency of a lumped approach with the link to physical theory and possibilities for more rigorous evaluation offered by a distributed model [*Beven et al.*, 1995].

TOPMODEL is based upon two basic assumptions: that the dynamics of the saturated zone can be approximated by successive steady state representations, and that the hydraulic gradient of the saturated zone can be approximated by the local surface topographic slope. A third assumption used in the original TOPMODEL, describes the distribution of downslope transmissivity with depth as an exponential function of depth to the water table. However, newer formulations of TOPMODEL allow this distribution to assume other mathematical functions that may be more appropriate for watersheds with complex baseflow recession curves [see *Ambroise et al.*, 1996].

The three assumptions above help derive a formula for the calculation of runoff from a catchment as a function of the topographic index. This topographic index is a measure of hydrological similarity among points within the catchment [*Beven et al.*, 1995; *Beven*, 1997]. All points with the same value of the index are assumed to respond in a hydrologically similar way. Therefore, it is not necessary to make calculations for all points in a catchment, only for different values of the index. High index values tend to saturate first and thus indicate potential subsurface or surface contributing areas. The expansion and contraction of those areas as the catchment wets and dries is then indicated by the pattern of the index. The spatial distribution of the topographic index may be derived from analysis of a digital elevation model (DEM) of the catchment using a computer program [*Quinn*, 1991]. More recent versions of TOPMODEL include the possibility of incorporating the spatial variability of soil hydraulic characteristics using a soil-topographic index to better represent the heterogeneity of both soil and hillslope form [*Beven*, 1986].

Additional components of a hydrological model such as interception, infiltration, evapotranspiration, flow routing, and snow accumulation and melt have been implemented in the TOPMODEL framework in different forms. TOPMODEL is primarily a simplified model of the saturated zone and its control of surface and

subsurface contributing areas, therefore those processes named above are not defined *a priori*.

TOPMODEL was originally developed to simulate small upland catchments in the United Kingdom, but has been applied with good results to numerous other catchments in humid temperate regimes in the eastern US, New Zealand, and Scotland. Applications to catchments in other parts of the world has been met with varied success, usually due to the violation of one or more of the assumptions of the model, in particular those of a quasi-parallel water table and a topographic control on water table depth. Other instances where model assumptions may be invalidated is for catchments where an infiltration-excess runoff mechanism is thought to be important. However, recent TOPMODEL developments reduce the restrictions of the model by simulating shallow subsurface and groundwater discharge as separate processes [*Scanlon et al.*, 2000] and by simulating the upslope contributing area dynamically [*Beven and Freer*, 2001].

Chapter 3

Material and Methods

3.1 Places of Study

3.1.1 Introduction

Although there is no field component to the study presented here, field data obtained by other researchers were used to test and validate the models developed for this study.

Annual records from 1982 to 1994 of maximum standing biomass of grasses and forbs at different nitrogen fertilization levels in the Cedar Creek Natural History Area in Minnesota [*Tilman, 1996*] were used for the evaluation of the one-dimensional grassland simulation model. Hourly hydrological records and distributed measurements of soil carbon and nitrogen from the Walker Branch Watershed [*Garten et al., 1994*] in Oak Ridge, Tennessee were used for the validation of the distributed model with respect to temperate forested catchments. Both sites have been the subject of numerous studies. Cedar Creek research has centered on plant diversity, effects of herbivores on grasslands, and nutrient studies, among others [*Gleeson and Tilman, 1994; Tilman, 1996; Wedin and Tilman, 1996*]. Research performed at Walker Branch Watershed includes many hydrological and biogeochemical investigations, among them: streamflow components, chemical budgets, stream nutrients, and soil

nitrogen [*Mulholland et al.*, 1990; *Mulholland*, 1992; *Genereux et al.*, 1993; *Garten et al.*, 1994; *Huston and Fontaine*, 1994].

3.1.2 Cedar Creek Natural History Area

The Cedar Creek Natural History Area (CCNHA) is a 2,185 ha (5,400 ac) experimental ecological reserve located at 45.4°N, about 50 km north of Minneapolis and St. Paul, Minnesota (<http://www.cedarcreek.umn.edu/>). It was established in 1940 and is one of the sites for Long Term Ecological Research (LTER) funded by the National Science Foundation.

Cedar Creek has a typical mid-continental climate with hot, humid summers and cold winters. Precipitation is spread fairly evenly throughout the year. Cedar Creek lies at the boundary between prairie and forest biomes. The terrain is a slightly undulating, with the uplands dominated by oak savanna, prairie, hardwood forest, pine forests, and abandoned agricultural fields and the lowlands comprised of ash and cedar swamps, acid bogs, marshes, and sedge meadows [*Hodson*, 1985]. Cedar Creek sits on a large glacial outwash sand plain and its soils are derived from it, spanning five of the ten soil orders. Upland soils are nitrogen poor.

3.1.3 Walker Branch Watershed

The Walker Branch Watershed (WBW) is a 97.5 ha (241 ac) forested catchment located at 36°N in the southeastern United States within the Ridge and Valley Province of the Appalachian highlands in Oak Ridge, Tennessee (<http://www.esd.ornl.gov/programs/WBW/>). The Walker Branch Watershed is within the Oak Ridge Reservation at the Oak Ridge National Laboratory.

It consists of two gaged catchments of first order streams, the east and west fork, which contain 59.1 and 38.4 ha (147 and 95 ac) respectively. The elevation ranges from 265 m at the confluence of the two streams, to 350 m at the crest of

Chestnut Ridge. The slopes average about 30 percent. Climate is typical of the southern humid Appalachian region and is classified as humid mesothermal. Both catchments are underlain by Knox dolomite, and soils are primarily Ultisols, with small areas of Inceptisols in alluvial locations adjacent to the streams [Elwood and Henderson, 1975; Genereux et al., 1993]. The soils are well drained and have a high infiltration capacity.

Prior to 1942 about 25 percent of the Walker Branch catchment area was cleared for agriculture. Since then the area has remained virtually undisturbed except for the establishment of a small, 2.5 ha (6.2 ac) plantation of loblolly pine. Figure 3 shows the historical landuse for the Walker Branch Watershed. The area supports an uneven-aged mature hardwood forest, mostly dominated by oak and hickory, with scattered pines on the ridges and tulip poplar and beech, near the stream channels [Johnson, 1989].

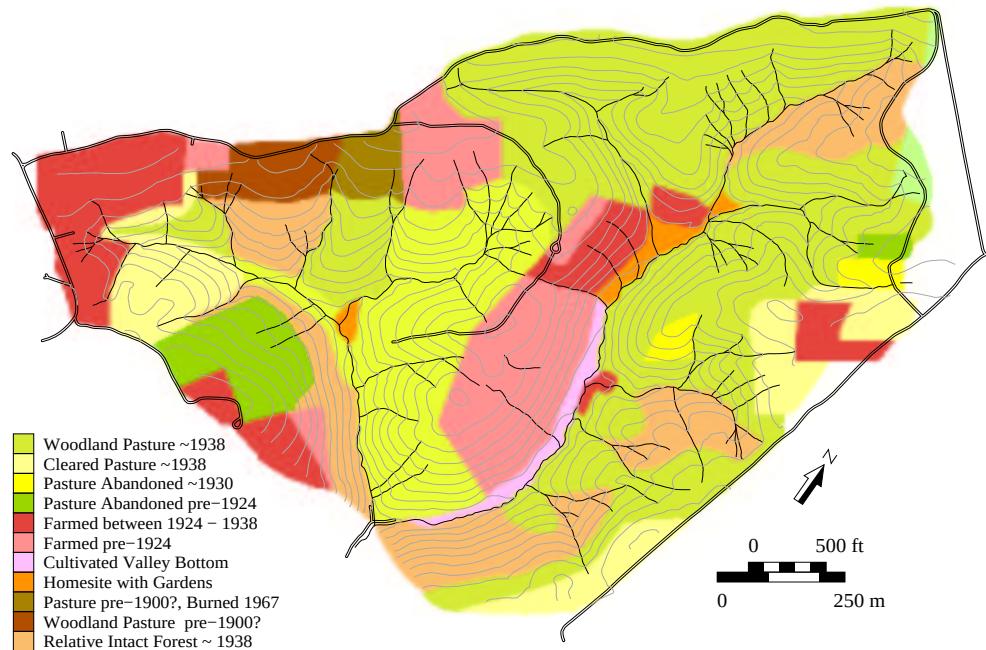


Figure 3: Walker Branch Watershed historical landuse [Huston, unpublished].

3.2 Biogeochemical Model

3.2.1 Introduction

The selection of a biogeochemical model for use in the present study was a difficult one. A large number of different biogeochemical models have been developed (see Section 2.2.2). However, for this study the interest was in a model that included both carbon and nitrogen dynamics in a process-oriented manner, and that at the same time was easily available and well tested. Furthermore, the model chosen should be applicable to small catchments.

3.2.2 Description of DNDC

The DeNitrification-DeComposition model (DNDC) of *Li et al.* [1992a, 1994a] was chosen as the best model for the purpose of this study. DNDC is a process-oriented simulation model of soil carbon and nitrogen biogeochemistry. DNDC version 6.7 was used in this study. Figure 4 shows the four interacting submodels (soil climate, plant growth, decomposition, and denitrification) that make DNDC.

The soil climate submodel is a one-dimensional soil heat flux and moisture flow model that calculates average hourly and daily soil temperature and moisture profiles. The soil is divided into a series of horizontal layers, and each layer is assumed to have a uniform temperature and moisture content, assigned to a point in the middle of the layer. The total soil depth is a user-defined parameter, with the thickness of the soil layers depending on the porosity and saturated hydraulic conductivity of the soil.

The water fluxes and heat flow between layers are determined by soil water potential and soil temperature gradients, and numerically modeled by explicit finite difference equations. All values are determined per unit area in the horizontal plane.

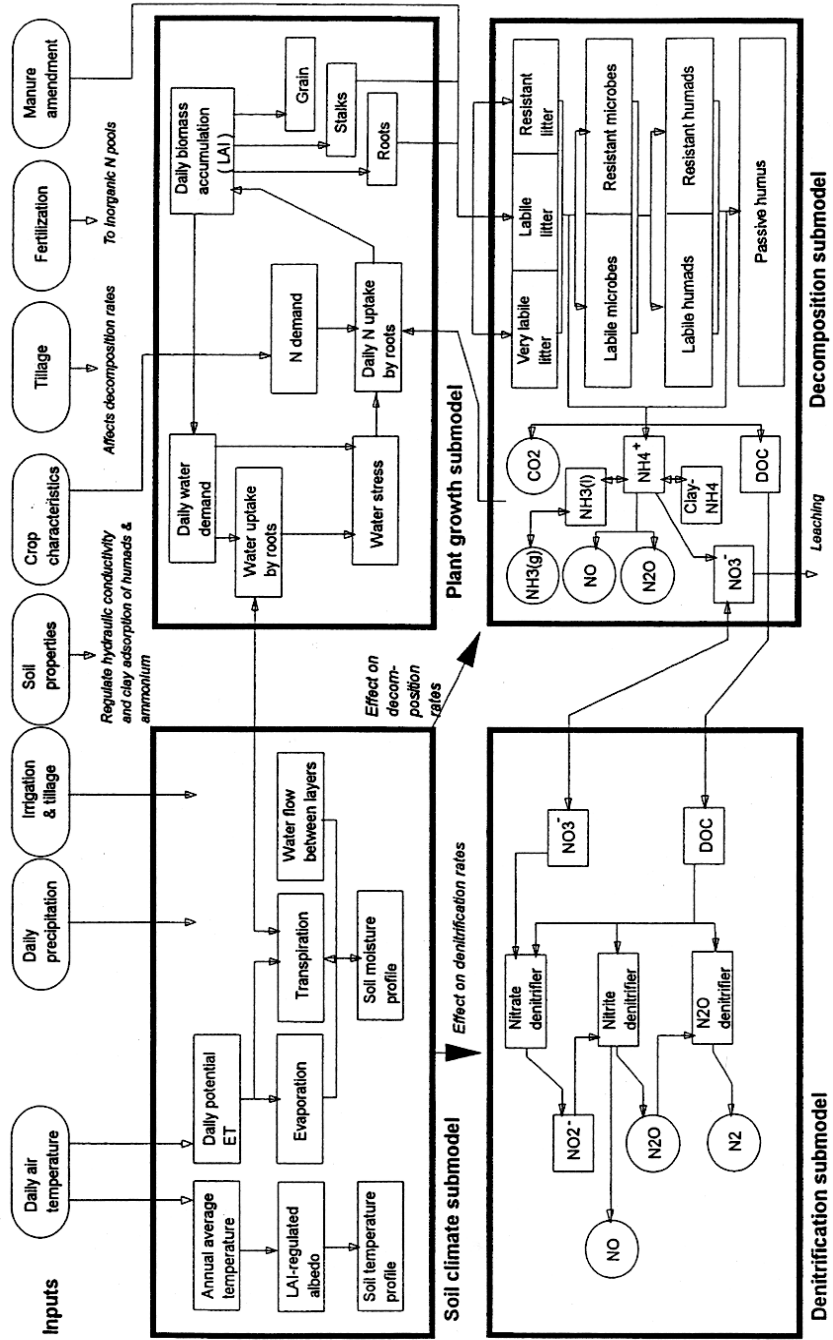


Figure 4: Schematic diagram of the DNDC model [from *Li et al., 1997*].

In DNDC, the flow of water between soil layers is described by Darcy's Law as in Equation 1:

$$Q_{i,i-1} = -K_{i,i-1} \cdot \frac{(h_i - h_{i-1})}{(z_i - z_{i-1})} \quad (1)$$

where:

$$h_i = \phi_i - z_i \quad (2)$$

and:

$$\phi_i = \begin{cases} \phi_{sat} \cdot \theta_i^{-\beta}, & \text{if } \theta < W_* \\ -m_1 \cdot (W_* - m_2)(W_* - 1), & \text{if } \theta \geq W_* \end{cases} \quad (3)$$

Water flow at the bottom of the soil profile is driven by gravity drainage only. DNDC assumes that all precipitation events start at midnight and are of constant intensity. Snowfall is generated if the air temperature during precipitation is less than or equal to 0°C. The snowpack grows with newly fallen snowfall as long as the air temperature stays at or below 0°C. Otherwise, snowmelt occurs at a rate of $0.0015 \times \text{air temperature}$. Canopy interception is modeled by an empirical equation of the leaf area index (LAI) defined by:

$$interception = \begin{cases} 0, & \text{if } store_{intcp} \geq store_{intcp_{max}} \\ 0.1 \cdot LAI \cdot precipitation, & \text{if } store_{intcp} < store_{intcp_{max}} \end{cases} \quad (4)$$

All the water that reaches the soil infiltrates, and saturates the soil starting from the top, layer by layer, to the depth that it can fill. Any residual rainwater not needed to fill a layer is uniformly distributed into the next deeper layer. A user-defined fraction of the water percolating from the bottom-most layer of the soil goes into a reservoir that empties only through transpiration, the rest of the percolating water flows into a deep groundwater reservoir and is lost to the system.

Evapotranspiration is calculated as monthly average values using the Thornthwaite formula shown in Equation 5.

$$PET = \begin{cases} 0, & \text{if } T_a < 0^\circ C \\ 16.2 \left(\frac{10T_a}{I} \right)^a, & \text{if } 0 \leq T_a < 26.5^\circ C \\ -415.85 + 32.24T_a - 0.43T_a^2, & \text{if } T_a \geq 26.5^\circ C \end{cases} \quad (5)$$

where:

$$I = \sum_{i=1}^{12} \left(\frac{T_{ai}}{5} \right)^{1.514} \quad (6)$$

and:

$$a = 6.75 \times 10^{-7} I^3 - 7.71 \times 10^{-5} I^2 + 1.79 \times 10^{-2} I + 0.49 \quad (7)$$

Potential transpiration is calculated separately, and is defined as a simple function of LAI, daily plant carbon uptake as a function of transpiration, and fixed daily plant water requirement (a multiplier that varies among species).

$$PT = 0.001 \cdot LAI + Plant_{water\ req.} \cdot Plant_{daily\ carbon} \quad (8)$$

Potential transpiration is divided equally among the soil layers, and if the total transpiration demand is not met from the soil layers, water is taken from a reservoir that simulates transpiration of deep rooted plants. Evaporation takes place from canopy interception storage, snowpack, and soil. Actual evapotranspiration from soil is decreased linearly to zero as the soil water potential drops from field capacity to wilting point. The sum of the transpiration and all the different evaporations constitutes the actual hourly evapotranspiration for the whole soil-plant system.

DNDC characterizes soil physical properties by soil texture into twelve classes (see Table 2), and representative parameters for each of the soil textures come from the work of *Clapp and Hornberger* [1978].

Table 2: Types of soil according to texture.

Soil Texture	Class Number
sand	1
loamy sand	2
sandy loam	3
silt loam	4
loam	5
sandy clayey loam	6
silty clayey loam	7
clay loam	8
sandy clay	9
silty clay	10
clay	11
organic	12

The gradient driven flux of soil temperature between layers is given by:

$$q_{i,i-1} = -k_{i,i-1} \cdot \left(\frac{T_i - T_{i-1}}{z_i - z_{i-1}} \right) \quad (9)$$

where the soil thermal conductivity k , depends on soil water content and on the type of soil (mineral or organic) as:

$$\begin{aligned} k_i &= (1 - n) \cdot k_{min} + n \cdot \theta_i \cdot k_{water} \\ k_i &= (1 - n) \cdot k_{org} + n \cdot \theta_i \cdot k_{water} \end{aligned} \quad (10)$$

Heat flux at the soil surface is simplified to a gradient-driven flux between the surface temperature, assumed to be equal to the mean air daily temperature (with a correction factor for latitudes below 40°), and the top soil layer temperature. The heat flux at the bottom of the soil profile is determined by the gradient between the bottom layer temperature and the annual mean air temperature imposed at 5 m depth.

The plant growth submodel calculates daily root respiration, nitrogen uptake by plants, and plant growth. Nitrogen uptake by vegetation is the key process in

DNDC linking crop growth with climate and soil status. The daily nitrogen uptake is regulated by four factors: the crop potential maximum yield, the crop carbon to nitrogen ratio (C:N), the crop growth curve, and the availability of dissolved inorganic nitrogen in the soil profile.

DNDC defines the crop potential maximum grain yield (PMGY) as the optimum grain yield of a crop growing with sufficient water and nitrogen. The model assumes that all other nutrients and light are always in adequate supply (i.e. they are not modeled). Values of PMGY for major crops are derived from the literature based on field production data.

The potential maximum biomass (crop) yield (PMBY) is calculated using the PMGY value and the fraction of the crop biomass carbon that is in the grain carbon pool at harvest (G_f):

$$PMBY = \frac{PMGY}{G_f} \quad (11)$$

From the PMBY value and the carbon to nitrogen ratio of the crop (a crop parameter), the crop potential maximum nitrogen uptake (PMNU) is obtained:

$$PMNU = \frac{PMBY}{C:N} \quad (12)$$

Daily optimal crop growth is determined using a generalized crop growth curve defined for all crops in terms of the fraction of the growing season elapsed (t_{fg})

as:

$$FG = \begin{cases} 8.878t_{fg}^{3.87}, & \text{if } t_{fg} > 0.3 \\ -0.660t_{fg} + 3.485t_{fg}^2 - 0.930t_{fg}^3 - 0.889t_{fg}^4, & \text{if } t_{fg} \leq 0.3 \end{cases} \quad (13)$$

The potential daily nitrogen uptake (N_{up}^*) is calculated as the difference between the optimal crop biomass nitrogen for that day and the actual nitrogen

content of the crop at the beginning of the same day (N_{crop}):

$$N_{up}^* = FG \cdot PMNU - N_{crop} \quad (14)$$

The actual daily nitrogen uptake is then calculated layer by layer down the soil profile, with the demand for nitrogen in each layer equal to the potential nitrogen uptake divided by the number of soil layers. DNDC tracks nitrogen in three different pools. Each pool corresponds to a form of inorganic nitrogen absorbed by plants, which are NO_3^- , NH_4^+ , and NH_3 . Ammonia (NH_3) is not directly absorbed by plants, but is extremely soluble in water and once dissolved it ionizes to NH_4^+ [Haynes, 1986]. The model does not discriminate against a particular form of nitrogen during uptake, all forms of inorganic nitrogen are absorbed in the proportion in which they are available. The availability of nitrogen to plants is dependent on the soil water solution concentration and soil moisture, as long as the temperature is above 0°C, otherwise nitrogen is not available.

DNDC keeps track only of the total crop-nitrogen uptake throughout the growing season. At the end of the growing season, the total crop biomass carbon is calculated as the product of the actual annual nitrogen uptake and the fixed crop C:N ratio. The total crop biomass is then partitioned into three pools: grain, roots, and shoots based on partitioning parameters specified in the crop files. After partitioning, all of the grain is removed from the soil-plant system, all of the roots stay in the soil, and the proportion of shoots left on the field depends on a user defined parameter of the model.

In this version of DNDC (v.6.7), root respiration is modeled as the result of only a root age factor that declines linearly as the plant goes from emergence to harvest, and the soil temperature several centimeters down. However, Li *et al.* [1994a] present a more elaborated root respiration for an earlier version of DNDC.

DNDC includes data for 28 major crops among them: corn, soybean, wheat, barley, sugarcane, alfalfa, cotton, and hay. The data for each crop consists of optimum yield, grain, root, and shoot proportions and C:N ratios, daily water requirements, maximum LAI, and maximum crop height.

The decomposition submodel of DNDC simulates the decomposition, assimilation, and loss processes that occur when the soil is in an aerobic state. During these processes, organic carbon, soluble carbon, NO_3^- and NH_4^+ are produced and may accumulate depending on the balance between the rates of mineralization, microbial biomass creation, and leaching and volatilization.

DNDC defines the total soil organic carbon as consisting of the sum of four carbon pools: decomposable residue (mainly plant residue), microbial biomass, humads (materials partly stabilized by humification and adsorption) and passive humus. The submodel utilizes the three active carbon pools for the decomposition sequence, which is performed layer by layer. The humus is assumed not to interact with the active phase of the soil organic matter.

Each active carbon pool has a labile and a resistant component, except for the residue pool that also has a very labile component. During decomposition each component of the three active pools decomposes independently via first order kinetics defined by:

$$\frac{dC}{dt} = \mu_{clay} \cdot \mu_{CN} \cdot \mu_{Tm} \cdot (S \cdot k_l + (1 - S) \cdot k_r) \quad (15)$$

A clay content reduction factor, μ_{clay} , is used in the equation, since the clay content of soils affects the decomposition of organic matter by adsorbing organic carbon and sheltering it from decomposition. μ_{CN} is introduced into the equation to reflect the limitations set by available nitrogen. Microbial biomass and residues have significantly different carbon to nitrogen ratios, therefore the actual decomposition depends on the amount of available nitrogen to balance that difference. DNDC

also models the effects of soil temperature and water content on microbial activity with a reduction factor, μ_{Tm} , that retards the decomposition rate for non optimum conditions. The specific decomposition rate, k , for each component was obtained from the literature on the production of carbon dioxide during decomposition experiments and adjusted to simulate field situations.

The production of microbial biomass is calculated as the product of the amount of CO_2 produced as the residue pools decompose and a microbial efficiency value that relates the ratio of carbon assimilated into microbial biomass to residue carbon release by decomposition. The microbial efficiency values in DNDC vary between 20 and 60 percent, depending if the soils are amended with easily decomposable organic material or not.

Microbial decomposition transfers 20 percent of the carbon to CO_2 , 60 percent to new microbial biomass, and the remaining 20 percent to the resistant humads pool. The resistant humads pool loses carbon through decomposition or tillage, and the carbon lost is distributed between the stable humus pool, CO_2 production, and new microbial biomass in a 40, 40, 20 percent proportion respectively. The soluble carbon pool is not actually a carbon pool but rather an indicator of the daily rate of decomposition. As such, it consists of the carbon from microbial biomass decomposition and humads decomposition that is recycled into microbial biomass.

In DNDC, nitrogen behavior during the decomposition of organic matter in the soil is simulated in three ways: nitrogen associated with carbon oxidized to CO_2 is transformed to NH_4^+ , nitrogen in NH_4^+ form can be nitrified to NO_3^- or transferred to NH_3 and volatilized to the air, and nitrogen from the transfer of organic carbon from one pool to another can create surpluses or deficits of available nitrogen because of the differences in C:N ratios among the different pools.

The inorganic nitrogen pool (NH_4^+ , NO_3^- and NH_3) collects nitrogen from the oxidation processes and supplies it for assimilation, nitrification, volatilization, denitrification, or plant uptake.

The decomposition submodel relates the volatilization of ammonia to the concentration of NH_3 in the liquid phase and a diffusion coefficient D :

$$AM = 2 \cdot NH_3 \cdot \left(\frac{D \cdot t}{3.14} \right)^{0.5} \quad (16)$$

During nitrification, NH_4^+ is oxidized to NO_2^- and NO_3^- . DNDC models the rate of nitrification as a function of the available NH_4^+ , soil temperature, soil moisture, and with an optimal rate at 35°C and soil pore moisture content of 90 percent:

$$dNNO = NH_4^+(t) \cdot [1 - e^{(-K_{35} \cdot \mu_{T,n} \cdot dt)}] \cdot \mu_{m,n} \quad (17)$$

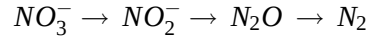
During nitrification the N_2O emission from the soil is correlated with the amount of nitrifiable nitrogen in the soil. DNDC models this process as a function of soil temperature and NH_4^+ concentration as:

$$N_2O = \frac{0.0014 \cdot NH_4^+}{30.0} \cdot \frac{(0.054 + 0.51 \cdot T)}{15.8} \quad (18)$$

Agricultural practices also affect the decomposition processes. DNDC models the following agricultural practices: crop rotation, tillage, fertilization, manure amendment, and irrigation. The crop rotation routine allows the sequential planting of different crops in a single field. Tillage simulates the changes in soil structure and aeration due to the application of plowing, disking, or mulching at different depths for conventional or conservation tillage. These changes include the uniform redistribution of residues, microbial biomass, humads, and passive humus over the tilling depth; the increasing of decomposition rates; the decreasing of soil moisture; the decreasing of the denitrifier population; and the conversion of resistant humads into

labile humads. The fertilization routine allows the addition of ammonium (NH_4^+), nitrate (NO_3^-), urea, and anhydrous ammonia to the soil system of at different depths. The fate of the fertilizers as they enter the soil is also modeled by DNDC. Farmyard manure additions are directly added to the labile, resistant, and humads residue pools at a set proportion. The addition of green manure is directly input to the fresh plant residue pool. Irrigation events are considered equivalent to rainfall events, with the same constant intensity, and the duration determined by the total volume of water added.

The denitrification submodel simulates the reduction sequence that takes place during denitrification:



DNDC activates the denitrification routine at every rainfall event and all denitrification calculations are performed layer by layer. DNDC assumes that denitrifying conditions (low oxygen availability) occur immediately upon saturation with water, that no decomposition takes place during denitrification, and that relative growth rates for different substrates are independent of each other.

Denitrification is carried out by denitrifiers capable of anaerobic growth only in the presence of NO_3^- , NO_2^- , or N_2O . Their growth rate is given by:

$$\left(\frac{dB}{dt}\right)_g = u_{DN} \cdot B(t) \quad (19)$$

u_{DN} is the relative denitrifier growth rate, and is calculated with double-Monod kinetics as:

$$u_{DN} = \mu_T \cdot (u_{\text{NO}_3} \cdot \mu_{p\text{HNO}_3} + u_{\text{NO}_2} \cdot \mu_{p\text{HNO}_2} + u_{\text{N}_2\text{O}} \cdot \mu_{p\text{HN}_2\text{O}}) \quad (20)$$

where the temperature reduction factor is:

$$\mu_T = \begin{cases} 2^{\frac{T-22.5}{10}}, & \text{if } T < 60^\circ\text{C} \\ 0, & \text{if } T \geq 60^\circ\text{C} \end{cases} \quad (21)$$

and the pH reduction factors are (in general, total denitrification decreases as soil pH decreases):

$$\begin{aligned} \mu_{pHNO_3} &= \frac{7.14 \cdot (pH - 3.8)}{22.8} \\ \mu_{pHNO_2} &= 1.0 \\ \mu_{pHN_2O} &= \frac{7.22 \cdot (pH - 4.4)}{18.8} \end{aligned} \quad (22)$$

The relative denitrifier growth for each substrate is defined from the maximum growth rate, the concentration of the substrate and soluble carbon, and half saturation constants for the substrate and the soluble carbon in the soil:

$$u_{N_xO_y} = u_{N_xO_y, \max} \cdot \frac{C}{K_{C, 1/2} + C} \cdot \frac{N_xO_y}{K_{N_xO_y, 1/2} + N_xO_y} \quad (23)$$

As the denitrifiers die, the carbon and nitrogen from the dead cells are added to the pools of immobilized carbon and nitrogen and no longer participate in the dynamic processes. However, this loss of carbon and nitrogen from the soil system is insignificant, since the denitrifiers biomass is a very small fraction of the total soil biomass. The denitrifier death rate is modeled as proportional to the denitrifier biomass as:

$$\left(\frac{dB}{dt} \right)_d = M_c \cdot Y_c \cdot B(t) \quad (24)$$

M_c and Y_c are two denitrification parameters, the first one is the maintenance coefficient on carbon, and the second one is the maximum growth rate on soluble carbon.

Competition among the denitrifying bacteria takes place via the common soluble carbon substrate. Soluble carbon is used by bacteria as the basic material for cell synthesis and energy. The rate of consumption of soluble carbon depends on the biomass, relative growth rate, and maintenance coefficients of the denitrifier populations. It is expressed as:

$$\frac{dC_{con}}{dt} = \frac{u_{DN}}{Y_c + M_c} \cdot B(t) \quad (25)$$

The carbon dioxide production is calculated as the difference between the total amount of carbon consumed and the amount used for cell synthesis:

$$\frac{dCO_2}{dt} = \frac{dC_{con,t}}{dt} - \left(\frac{dB}{dt} \right)_g \quad (26)$$

As denitrifiers grow they consume substrate. The rate of this consumption is given by:

$$\frac{dN_xO_y}{dt} = \left(\frac{u_{N_xO_y}}{Y_{N_xO_y}} + \frac{M_{N_xO_y} \cdot N_xO_y}{N} \right) \cdot B(t) \cdot \mu_{pHN_xO_y} \cdot \mu_T \quad (27)$$

The maintenance coefficients reported in the literature are for the entire denitrifier biomass, since DNDC calculates the consumption for each of the three substrates, the maintenance coefficient $M_{N_xO_y}$ has to be multiplied by the relative presence of each electron acceptor in the water phase.

Once the growth rate and the C:N ratio of the denitrifiers are known, the rate of nitrogen assimilation during denitrification can be calculated as:

$$\left(\frac{dN}{dt} \right)_{asm} = \left(\frac{dB}{dt} \right)_g \cdot \frac{1}{CNR} \quad (28)$$

The C:N ratio of the denitrifiers is based on the chemical composition reported for *Paracoccus denitrificans* ($C_6H_{10.8}N_{1.5}O_{2.9}$).

The daily emissions of the resulting products of denitrification are calculated by the model as functions of the adsorption coefficient of the gases in soils and the air filled porosity of the soil:

$$P_{N_2} = 0.017 + (0.025 - 0.0013 \cdot AD) \cdot PA \quad (29)$$

$$P_{N_2O} = (0.0006 + 0.0013 \cdot AD) \cdot (0.013 - 0.005 \cdot AD) \cdot PA \quad (30)$$

DNDC assumes that denitrification is concentrated in the surface soil, therefore, the effect of soil depth on diffusion is not considered.

3.2.3 Improvements to DNDC

Section 3.2.2 presented a description of the DNDC model in its original form. This section shows the improvements, modifications, and additions to DNDC by the author of this study for increasing its process-based capabilities and allowing its linkage to a hydrological model (see Section 3.4).

The original form of DNDC was completely recoded into PV-WAVE v.7.01 [Visual Numerics, 2000]. PV-WAVE is an easy-to-use, array-oriented, fourth generation programming language capable of performing complex analysis, visualization, and application development quickly and interactively.

Once the original form of DNDC was implemented in PV-WAVE, it was intensively tested against the original coding of DNDC to verify that all results were identical, except for rounding errors. The new version of DNDC (PV-WAVE version) was tested with different types of crop, soils, climate, and other input parameters. In all cases, both versions of DNDC delivered identical results.

As shown in Section 3.2.2, DNDC consists of four submodels: soil climate, plant growth, decomposition, and denitrification. In broad terms, the changes to DNDC consisted of redoing the plant growth submodel, improving several routines

in the soil climate submodel, additions to the decomposition submodel, and slight modifications to the denitrification submodel.

The plant growth submodel of the original DNDC utilized a generalized optimal growth curve to determine the daily growth of any crop and its corresponding nitrogen requirement (see Section 3.2.2). This approach at obtaining crop growth is not mechanistic. It assumes that all crops follow the same fixed growth pattern regardless of environmental conditions.

In the new version of DNDC, optimum plant growth depends on previous day growth, daily growth rate, C:N ratio of leaves, and environmental conditions as:

$$plant\ growth_i = plant\ growth_{i-1} \cdot DI \cdot CN_{i-1} \cdot EnvC_i \quad (31)$$

This approach to plant growth follows *Wu et al. [1994]*, where growth is estimated as a function of interacting growth factors. Each of the three growth factors (daily growth rate, C:N ratio of leaves, and environmental conditions) is defined as an index that varies between zero and one.

The daily growth rate factor is a simple step function that reduces the daily potential relative growth rate of a plant according to the amount of precipitation. It is a surrogate of the negative effect of cloud cover on solar radiation, and therefore on growth, since the model does not simulate photosynthetic processes directly. The daily potential relative growth rate is a measure of the amount of growth that a plant is capable of achieving in a day when all the environmental factors are not limiting [*Grime and Hunt, 1975; Charles-Edwards et al., 1986; Hunt, 1990*]. Each species of plant has its own characteristic daily potential relative growth rate.

In nature, the C:N ratio of leaves varies depending on the amount of nitrogen available in the soil for plant uptake. Nitrogen is a limiting nutrient, while carbon is usually in ample supply for plant growth. To simulate this behavior, we follow an approach similar to *Parton et al. [1988]*, where the C:N ratio of a plant is

allowed to vary only within certain range. As the C:N ratio of the leaves gets higher than a plant optimal ratio, the CN_l index factor (see Equation 31) is lowered with the corresponding reduction in plant growth. The plant C:N ratio is calculated from the carbon allocated to leaves from Equation 31 and the nitrogen uptaken from the soil allocated to leaves. The allowable range of C:N variation follows an S-shaped curve function. S-shaped curves are seen often in nature because they are a fairly good abstraction of the course of a self-limiting process such as the growth of an organism in a limited environment.

Environmental conditions limit the growth of plants [Chapin *et al.*, 1987]. DNDC uses Liebig’s law of the minimum [Barbour *et al.*, 1999] to determine the more limiting of the environmental conditions modeled. Soil moisture, soil temperature, and air temperature are the environmental parameters limiting growth in DNDC. Each one of these three environmental conditions is calculated as an index varying in value from zero to one. The soil moisture index is determined by an S-shaped curve of plant growth response to soil water. Dry and wet days are also tallied to simulated physiological status and delayed adjustment due to dry conditions. The soil temperature index is calculated as a linear relationship of soil temperature and a zero-to-one index. A soil temperature of 10° C or above will not limit growth (the index would be equal to one), and below 1°C growth stops. The air temperature index is calculated as a set of linear relationship with breakpoints at specified temperatures. Below an air temperature of 2°C no growth occurs, maximum growth increases linearly until 25°C, and above an air temperature of 25°C growth decreases again. Soil moisture and temperature are estimated at different soil depths.

Optimum plant growth is also limited by the actual daily plant transpiration rate. Plants uptake CO₂ for photosynthesis by opening their stomata, allowing the passage of water vapor from the interior of the leaf to the surroundings. If the plant is unable to take up enough water from the soil for this transpiration process,

water stress develops, and the plant eventually closes its stomata reducing greatly the water loss and the CO₂ uptake [*Aber and Melillo, 1991; Larcher, 1995*]. This water loss-carbon gain relationship is expressed as the water use efficiency (WUE) of photosynthesis and its value has been calculated for different types of plants. WUE is implemented in the model by limiting the optimum plant growth to that of the actual daily transpiration times its WUE.

In the new version of DNDC, growth starts with translocation of nutrients from seed or roots depending on the type of plant in question (annual, herbaceous perennial, or woody perennial). The translocation of resources from storage organs in the plant allows the plant to begin its growing cycle [*Hayes, 1985; Aber and Melillo, 1991*]. In the model, the translocation lasts for two weeks, and the amount of nutrients transferred are a percentage of the nutrients stored in the plant during the dormant season up to a maximum amount. Environmental conditions also limit the transfer of nutrients during translocation. The onset of the translocation is given by the start of the growing season as determined by cumulative degree-days. Initial leaf emergence in plants has been found to relate well to cumulative degree-days [*Baskerville and Emin, 1969; Lechowicz, 1984*]. The new version of DNDC uses the simple average method to determine cumulative degree-days, with each plant species having a characteristic minimum threshold air temperature for starting accumulating degree-days and a minimum cumulative degree-days for starting growth:

$$CDD = \sum_{d=1}^{d_g} \begin{cases} 0, & \text{if } T_{air} \leq T_{plant_{thld}} \\ T_{air} - T_{plant_{thld}}, & \text{if } T_{air} > T_{plant_{thld}} \end{cases} \quad (32)$$

In DNDC, actual plant growth depends on the amount of nitrogen a plant can extract from the soil solution given a predetermined demand for nitrogen. The new version of the model calculates this demand by using Equation 31. The uptake routine has also been changed in the new version, the demand is met from the top

layer of soil down to the lower layers. If all the demand for nitrogen is achieved at the top layer, the rest of the layers do not supply any nitrogen. However, if after extracting all the available nitrogen from all the layers there still is some demand left, the model adds this deficit of nitrogen to next day's demand. Therefore, poor growth due to suboptimal conditions early in the season can be recovered by optimal conditions later.

Nitrogen uptake in the model is also a function of the root mass index. This index is defined as a Michaelis-Menten function of the root mass for every layer with respect to an initial root mass. The Michaelis-Menten equation is a type of S-shaped curve widely used to represent self-limiting processes in ecology [*Fitter and Hay, 1987*].

The root distribution and growth routine allocates root growth according to the amount of nutrients in each layer. Roots cannot grow deeper than the thickness of the soil defined in DNDC, typically 0.5 m. However, this depth encompass a large percentage of the roots in temperate ecosystems [*Bartos and Jameson, 1974; Jackson et al., 1996; Jobbagy and Jackson, 2000*]. The initial root distribution follows the model of *Gerwitz and Page [1974]*. Root mortality is implemented as a constant daily proportion of the root carbon (0.44% per year [*Head, 1973*]) that doubles when daily soil moisture is at or below the wilting point. Trunk mortality for woody perennials is simulated in a similar way (1.5% per year of the trunk carbon [*Edwards et al., 1989*]).

The new version of DNDC, partitions plant biomass growth into roots, shoots (leaves and trunk), and grains each day. The previous version performed the partition only at harvest time and at a fixed proportion. The allocation of biomass to different parts of a plant is a complex process not completely understood [*Monk, 1966; Thornley, 1972; Nadelhoffer et al., 1985; Chapin et al., 1987; Wilson, 1988; Garnier, 1991*]. DNDC allocates biomass differently depending on the type of plant.

For annual plants, the model allocates most growth to leaves until grain production time, when all growth is transferred to grains. In herbaceous perennials, a large percentage of the growth is allocated to roots until an optimum root:shoot ratio is reached, then growth is mostly directed to leaves unless the plant is under nitrogen stress (not enough nitrogen in the soil), when roots take up a large proportion of the growth. Woody perennials growth is allocated to leaves until an optimum value is achieved, most allocation is then switched to roots until the initial root mass is reached, when most growth is directed toward the trunk.

The adsorption of ammonium by soil clay and organic matter is an important process in plant growth. NH_4^+ is held by the negatively charged surfaces of clay and organic matter in exchangeable form, available for plant uptake, but partially protected from leaching [*Brady and Weil, 1999*]. This process maintains the nutrients in the soil, where plants can take them, but away from the soil solution. After irrigation or a storm, the soil solution may percolate down to the groundwater carrying with it the plant nutrients. DNDC simulates ammonium adsorption as a function of the cation exchange capacity of the soil, and the amount of clay and organic matter in the soil:

$$\text{NH}_{4\text{ads}}^+ = \text{CEC} \cdot \frac{\text{clay} + \text{SOM}}{(\text{clay} + \text{SOM}) + 0.015} \quad (33)$$

Soil organic matter is calculated in the new version of DNDC by adding the amount of carbon in the litter and humus pools, and assuming that organic matter consists of 58 percent by weight of carbon. The upper value for soil organic matter in the model is 15 percent, except in the case of organic soil.

Several routines in the soil climate submodel of DNDC were also modified. In the soil climate submodel, Equation 5 describes the potential evapotranspiration formula of Thornthwaite. The formula is based on a standard month of thirty days, and twelve hours of sunlight [*Dunne and Leopold, 1978; Xu and Singh, 2001*], but

it was not adjusted in the original version of the model. Therefore, the new version adjusts PET for the number of days in the month, and the hours of sunlight during the day according to:

$$PET = PET' \cdot \frac{N_{month}}{30} \cdot \frac{H_{day}}{12} \quad (34)$$

where:

$$H_{day} = 7.64 \cdot \arccos \left(\frac{\sin \left(\frac{2\pi}{360} \cdot \phi_{lat} \right) \cdot \sin(sun_d) - 0.044}{\cos \left(\frac{2\pi}{360} \cdot \phi_{lat} \right) \cdot \cos(sun_d)} \right) \quad (35)$$

and:

$$sun_d = 0.4102 \cdot \sin \left(\frac{2\pi}{days_{year}} \cdot (days_{elapsed} - 80.25) \right) \quad (36)$$

Hamon method for determining PET was also incorporated in the new version of DNDC. Hamon formula [[Hamon, 1961](#); [Jensen et al., 1990](#); [Xu and Singh, 2001](#)] for determining potential evapotranspiration is also temperature based, but it was developed from measurements taken in Southern Appalachia, which makes it more applicable than Thornthwaite formula to the study site at Walker Branch Watershed (see Section [3.1.3](#)):

$$PET = 0.55 \cdot H_{day}^2 \cdot Pt \quad (37)$$

where:

$$Pt = \frac{4.95 e^{(0.062 \cdot T_{air})}}{100} \quad (38)$$

H_{day}^2 is the hours of daylight for a given day and T_{air} is the daily mean air temperature.

The potential transpiration was reformulated according to Campbell relationship for the partitioning of evapotranspiration [[Campbell, 1985](#)]:

$$PT = PET \cdot (1 - e^{-0.82 \cdot LAI}) \quad (39)$$

LAI is now a simple function of leaf biomass, with an upper limit given by the plant maximum LAI:

$$LAI = 0.0008 \cdot leaf\ biomass \quad (40)$$

A new routine was incorporated to allow for the variation of field capacity and wilting point with changes in the soil organic matter. Soils high in organic matter have significantly higher available water capacity (field capacity–wilting point) than soils of similar texture that contain less organic matter [*Hudson, 1994; Brady and Weil, 1999*]. This new routine uses the linear equations of *Hudson [1994]* to determine the changes in field capacity and wilting point with organic matter for different types of soil.

The water delivery section of the soil climate submodel was adjusted so that evaporation takes places from all soil layers, and is not dependent on only one soil depth.

Several parts of the decomposition submodel were modified. The original routine determining the effect of temperature and moisture on decomposition was not correct. This routine is based on data from *Nyhan [1976]* and *Clay et al. [1985]*, but the original polynomial equations did not fit the data well. The old version of DNDC overestimated the effects of temperature and moisture on decomposition, except for low moisture values, which were underestimated. New polynomial equations, with good data fit, were generated and added to the routine. The decomposition of surface litter was modified to allow for the slow decomposition of vegetation left on the soil surface. Previously, the decomposable material was leaching NH_4^+ very rapidly. The original root litter routine allocated dead roots for decomposition according to a fixed proportion. More dead roots were apportioned to top layers of soil, less to lower layers. This routine was changed to fit the new root distribution. Now, each soil layer has a dynamic amount of roots, and the roots start decomposing in that

layer when death occurs. The distribution of soil organic matter was modified to accept a thicker soil profile, previously it was limited to 0.3 m.

Only one routine was modified in the denitrification submodel. The denitrification in frozen soil was not allowing the nitrogen gases to diffuse during the whole day, only for one hour. The routine was amended, so it resembles the other two denitrification formulations; denitrification during rainfall events and denitrification during periods of flooding.

The changes performed make this new version of DNDC a more mechanistic soil organic carbon model by improving both the plant growth component and the belowground nitrogen and carbon dynamics.

3.3 Hydrological Model

3.3.1 Introduction

The emphasis of this study is on a better description of the dominant spatial patterns of soil organic matter, nutrients, and hydrology at the small catchment level, rather than a more precise description of these same variables at any given point. Therefore, of all the hydrological models described in Section 2.3, a simpler, semi-distributed model is better suited for this study. A semi-distributed model is capable of fast computation of hydrological variables, while allowing output to be distributed in the spatial domain. The increased complexity and computing overhead of a comprehensive, distributed model is not warranted for this study.

3.3.2 Description of TOPMODEL

TOPMODEL is the only widely available semi-distributed parameter model for watershed hydrology. This study utilized the version of TOPMODEL by *Clapp et al.* [1992], which is based on the extensions made to TOPMODEL by *Hornberger et al.* [1985]. The central idea in TOPMODEL is that topography exerts a dominant

control on flow routing through upland catchments. Hence, TOPMODEL simulates runoff based on the variable source area concept of streamflow generation [Wolock, 1993]. The use of natural isotopes data to separate discharge hydrographs into old and new water has shown that the mechanisms of variable source area flow control most of the runoff in vegetated humid temperate catchments [Beven, 1986]. Three mechanisms constitute the variable source area concept: saturation overland flow from direct precipitation on saturated land surface areas, saturation overland flow from return flow of subsurface water to the surface in the saturated areas, and subsurface stormflow (interflow). Figure 5 shows an schematic diagram of the TOPMODEL concept.

In TOPMODEL, total streamflow is the sum of saturation overland flow and subsurface flow (q represents flow per unit area):

$$q_{total} = q_{overland} + q_{subsurface} \quad (41)$$

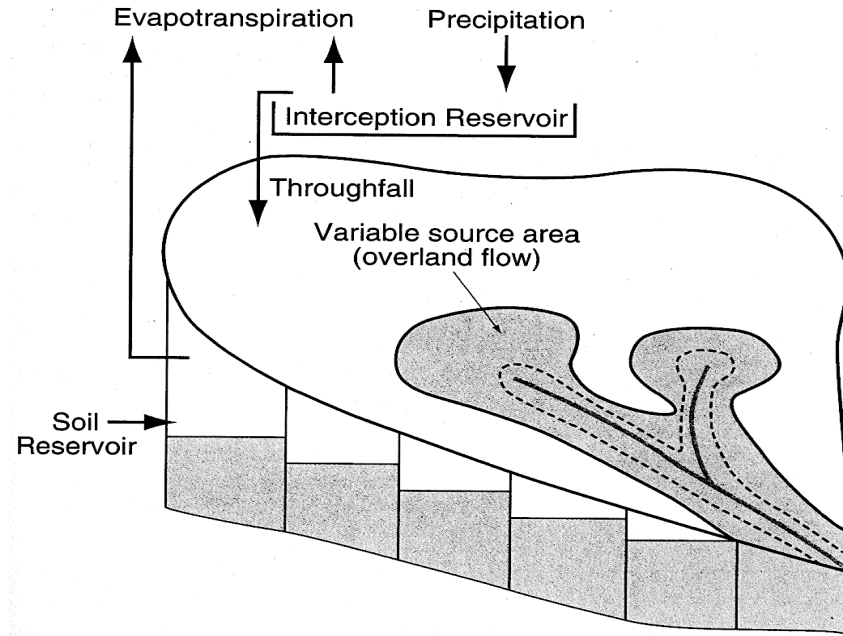


Figure 5: Diagram of the TOPMODEL concept [from Hornberger et al., 1998].

Saturation overland flow is the sum of direct precipitation on saturated areas and return flow:

$$q_{overland} = q_{direct} + q_{return} \quad (42)$$

To derive expressions for computing the specific flows, the continuity equation for a hillslope segment and Darcy's law are used. Assuming steady-state conditions (*in flow = out flow*) and a spatially uniform recharge rate (R) to the water table of the hillslope segment shown in Figure 6:

$$A \cdot R = T \cdot c \cdot \tan \beta \quad (43)$$

where, A is the surface area of the hillslope slice, T is the transmissivity of the soil, c is the contour width (length perpendicular to the flow direction), and $\tan \beta$ is the slope of the land surface. The slope of the of the water table is assumed to be the same as that of the land surface. The transmissivity of the saturated thickness is computed by assuming that the saturated hydraulic conductivity (K_z) decreases exponentially with depth:

$$K_z = K_0 \cdot e^{-fz} \quad (44)$$

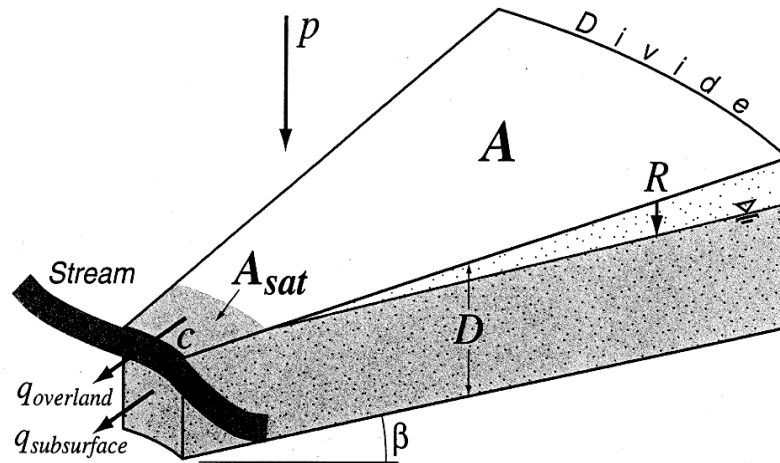


Figure 6: Water balance for a catchment hillslope [from *Hornberger et al., 1998*].

where K_0 is the hydraulic conductivity at the soil surface and f is a parameter that governs the rate of decrease of K with depth.

The transmissivity of the saturated zone from a depth of water table z_{wt} to a depth to bedrock z_D is given by:

$$T = \int_{z_{wt}}^{z_D} K_0 \cdot e^{-fz} dz \quad (45)$$

or:

$$T = \frac{K_0}{f} (e^{-fz_{wt}} - e^{-fz_D}) \quad (46)$$

The term e^{-fz_D} is generally much smaller than the term $e^{-fz_{wt}}$ [*Wolock, 1993*] so the equation can be simplified to:

$$T = \frac{K_0}{f} e^{-fz_{wt}} \quad (47)$$

TOPMODEL keeps track of the saturation deficit to do water balance accounting. The saturation deficit is the amount of water needed to be added to the soil at a given point to bring the water table to the surface. To set Equation 47 in terms of the saturation deficit, z_{wt} is replaced by $\frac{s}{\phi}$ where s is the saturation deficit and ϕ is the fraction of porosity of the soil:

$$T = \frac{K_0}{f} e^{-f \frac{s}{\phi}} \quad (48)$$

To simplify the notation, $\frac{K_0}{f}$ is defined as T_{max} , because this term is the transmissivity when the soil is completely saturated, and replace $\frac{f}{\phi}$ with $\frac{1}{m}$, a scaling parameter:

$$T = T_{max} e^{-\frac{s}{m}} \quad (49)$$

substituting Equation 49 into Equation 43:

$$A \cdot R = T_{max} e^{-\frac{s}{m}} \cdot c \cdot \tan \beta \quad (50)$$

solving for s , with $a = \frac{A}{c}$:

$$s = m \cdot \ln \left(\frac{R}{T_{max}} \right) - m \cdot \ln \left(\frac{a}{\tan \beta} \right) \quad (51)$$

Until this point, the equations have referred to an individual catchment hillslope, defined by a pair of streamlines and extending from the stream to the catchment divide (see Figure 6). To solve for the catchment average saturation deficit, Equation 51 is integrated over the catchment and divided by the area:

$$\bar{s} = \frac{1}{A} \int_A s \, dA \quad (52)$$

assuming R and T_{max} are constant over the catchment:

$$\bar{s} = m \cdot \ln \left(\frac{R}{T_{max}} \right) - m \cdot \frac{1}{A} \int_0^A \ln \left(\frac{a}{\tan \beta} \right) di \quad (53)$$

defining λ as the mean $\ln \left(\frac{a}{\tan \beta} \right)$ (topographic index) for the catchment and combining Equation 53 with Equation 51:

$$s = \bar{s} + m \cdot \left[\lambda - \ln \left(\frac{a}{\tan \beta} \right) \right] \quad (54)$$

Equation 54 is the fundamental TOPMODEL equation. It describes the saturation deficit at any point in the catchment as equal to the average saturation deficit for the catchment plus a soil parameter, m , times the difference between the average topographic index and the local topographic index.

The topographic index, $\ln\left(\frac{a}{\tan\beta}\right)$, quantitatively captures the effect of topography on the development of saturation areas in a catchment. A map of topographic indices for a catchment, calculated from the DEM of the catchment, shows areas where runoff processes such as saturation-excess overland flow are likely to occur. High values of the topographic index indicate areas with large contributing areas and relatively flat slopes, typically at the base of hillslopes and near the stream. Low topographic index values are found at the tops of hills, where there is relatively little upslope contributing area.

Equation 54 is used to determine the overland flow (see Equation 42). Direct runoff flow is generated when precipitation falls on a saturated area:

$$q_{direct} = \frac{A_{sat}}{A} \cdot P \quad (55)$$

$\frac{A_{sat}}{A}$ is calculated by computing s at any point. If s is less than or equal to zero, the soil is completely saturated and any rain on the surface will become direct overland flow. This occurs most easily for points within the catchment where the topographic index is large (cf. Equation 54). Return flow occurs where s is less than zero. The rate of the return flow is given by:

$$q_{return} = |s| \cdot \frac{A_{sat}}{A} \quad (56)$$

The other term of Equation 41, $q_{subsurface}$ is computed by combining Darcy's law for saturated subsurface flow (the right-hand side of Equation 43 divided by c) with Equation 49, the expression for transmissivity of the saturated thickness:

$$q_{subsurface} = T_{max} e^{-\frac{s}{m}} \cdot \tan\beta \quad (57)$$

To compute the mean subsurface discharge, $q_{subsurface}$ is integrated along the length of all stream channels and divided by the catchment area:

$$\bar{q}_{subsurface} = \frac{\int_L (T_{max} e^{-\frac{s}{m}} \cdot \tan \beta) dL}{A} \quad (58)$$

or:

$$\bar{q}_{subsurface} = T_{max} e^{-\lambda} e^{-\frac{s}{m}} \quad (59)$$

The equations presented in this section constitute the main conceptual points of the TOPMODEL framework. As explained in Section 2.3.3, TOPMODEL is a set of conceptual tools that can be used to simulate hydrological processes in a relatively simple way. Other components of a hydrological model, like evapotranspiration, interception, etc. are not defined *a priori*.

The temporal resolution of TOPMODEL is not fixed. The processes in the model can be simulated at any time step. However, the temporal resolution of the data needs to match the time scale of the dynamics in the theoretical framework of the model, and this time scale is thought to be in the order of hours [Wolock, 1993].

3.4 Linkage of TOPMODEL and DNDC

TOPMODEL simulates the spatial distribution of water in a catchment. DNDC models soil biogeochemistry, including plant growth, in one dimension — vertically. The linkage of these two models allows for the spatial distribution of the one-dimensional DNDC processes by running multiple instances of DNDC in a catchment, one for each of the TOPMODEL topographic index classes. In TOPMODEL, areas with the same topographic index have the same hydrological behavior (see Section 2.3.3). Figure 7 shows how DNDC is nested within TOPMODEL for the linked model. TOPDNDC is the name of the new model that links the processes of TOPMODEL and DNDC.

that does not allow water to infiltrate rapidly. This is for the stabilization of the finite difference algorithm used in the calculations.

Both TOPMODEL and DNDC calculate water fluxes. However, TOPMODEL is a purely hydrological model and has been used previously to model streamflow in the area of interest with good results [see *Huston and Fontaine, 1994*]. Therefore, in the linked model TOPDNDC, the TOPMODEL component handles all the hydrological processes.

The first step in linking these two models involves the decoupling of the hydrological routines of DNDC from the rest of the DNDC model. The parameters generated by the hydrological part of DNDC and utilized in the rest of DNDC are daily throughfall (water reaching the topsoil), daily percolated water per layer, daily soil water per layer, hourly water content per layer, and daily snow-pack. These parameters are now generated from the hydrological processes in the TOPMODEL component of TOPDNDC, and then input into the DNDC component. The DNDC component in TOPDNDC does not include any hydrological processes.

Output from the TOPMODEL component of TOPDNDC allows the generation of four of the five hydrological parameters required by DNDC. The fifth parameter, daily snow-pack, is not implemented in the version of TOPMODEL currently used and, therefore, is not available to the DNDC component of the model. However, the snow-pack and snow-melt processes in the Walker Branch Watershed (see Section 3.1.3), the area of interest for application of this model, have a negligible influence in its hydrological regime.

The other hydrological parameters are generated as follows. Hourly throughfall is calculated in TOPMODEL by subtracting the canopy interception and soil litter interception from every precipitation event. Throughfall is then accumulated for 24 hours and converted to duration units by assuming a constant precipitation intensity of 5 mm/hr. Hourly percolated water per layer is a direct output of the

TOPMODEL unsaturated zone fluxes. It represents water in excess of the root zone saturation. TOPDNDC assumes that the percolated water is distributed equally among the different DNDC soil layers. The percolated water is accumulated to daily values before passing it to the DNDC component. The daily soil water per layer and the hourly water content per layer are taken directly from the root zone area value in the TOPMODEL component. The TOPMODEL root zone is scaled to that of DNDC since the two root depths have different values. In TOPMODEL the effective root zone depth is given by *Beven* [2001] as:

$$Z_{rz} = \frac{S_{rmax}}{\theta_{fc} - \theta_{wp}} \quad (60)$$

where θ_{fc} is the soil moisture content at soil capacity, θ_{wp} is the soil moisture content at wilting point, and S_{rmax} is the maximum available root zone storage.

In DNDC the root zone depth is an input parameter. The scale factor is given by the ratio of the two rooting depths. The daily soil water per layer is the value of TOPMODEL root zone layer at the end of the day times the scaling factor divided by the number of soil layers in the DNDC component divided by the layer porosity. This last division converts the amount of water in the layer into the percentage of porous space filled with water within the layer, which is the required DNDC parameter. The hourly water content per layer consists of all the hourly root zone values for the day scaled to the ratio of the root depths and divided by the number of soil layers in the DNDC component.

The only parameter passed from DNDC back to the TOPMODEL component is leaf area index (LAI), and it is used to determine the amount of canopy interception.

Chapter 4

Results and Discussion

4.1 Results

4.1.1 Introduction

The results presented here are divided into two sections. The first section contains the results of the DNDC model (lumped model), applied to data from the Cedar Creek Natural History Area (see Section 3.1.2). The second section shows the results of the linked TOPDNDC model (distributed model) to data from the Walker Branch Watershed (see Section 3.1.3).

4.1.2 Lumped Model

4.1.2.1 Measured Data and Input Parameters

The field data collected at the Cedar Creek Natural History Area consist of 13 years of annual, maximum, standing biomass gathered from 207 grassland plots under eight different nitrogen addition rates.

The rate of nitrogen addition was 1.0, 2.0, 3.0, 4.4, 6.4, 10.5, 18.0, and 28.2 $g \cdot m^{-2} \cdot yr^{-1}$, including 1.0 $g \cdot m^{-2} \cdot yr^{-1}$ of nitrogen via natural atmospheric deposition. The nitrogen was added in equal amounts in early spring (approximately May 1) and early summer (approximately June 23) of every year, except for the nitrogen from atmospheric sources that was deposited throughout the year. For a detailed

description of the methods utilized to collect these data, its analysis and critique, see *Tilman* [1996]; *Huston* [1997]; *Tilman et al.* [2001].

The period of record of the field data encompassed years of great climatic variability, including a major drought in 1987 and 1988. This drought was the third worst drought of the past 150 years in the Cedar Creek area, as can be seen in Figure 8, which shows the Palmer Drought Severity Index (PDSI) in the last 30 years for East Central Minnesota (National Climatic Data Center (NCDC) Climate Division 6), where Cedar Creek is located. The PDSI provides standardized measurements of soil moisture conditions for comparison between locations and times. Its calculation is based on a monthly water balance, and the output from the calculation is an index value ranging from -4 (extreme drought) through 0 (normal conditions) to +4 (extreme wet period) [*McMahon*, 1993].

The 1988 growing season was also the hottest of the data collection period. There were also unusually cool growing seasons, 1992 and 1993, with several late

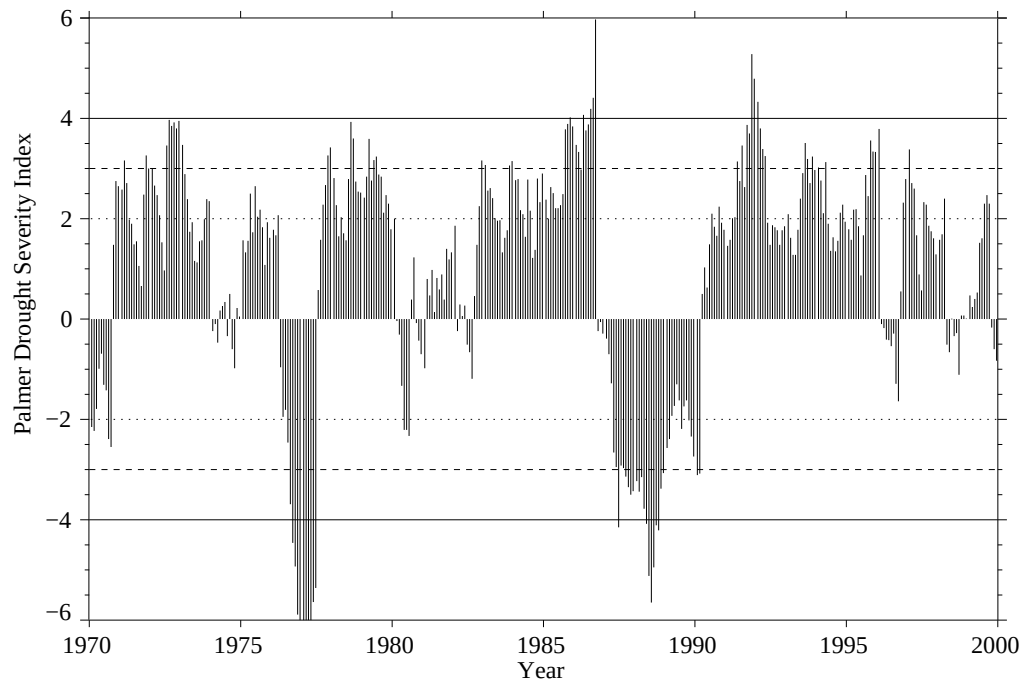


Figure 8: East Central Minnesota Palmer Drought Severity Index.

spring frosts, and in 1990 an unusually wet growing season but with normal temperatures. The first five growing seasons, 1982-1986, had near normal precipitation and temperatures.

Table 3 and Figure 9 show the values of the field data collected at grassland plots in the Cedar Creek Natural History Area during 13 years. The data consist of the summed dry mass of all aboveground living vascular plant species from a harvest at the peak of the growing season (approximately August 20) of each year. Each plot contained a different number of species of grasses and forbs. The number of species in each plot was inversely proportional to the amount of nitrogen added to that plot. This effect of decreased plant diversity at higher levels of productivity is a well-known ecological effect presumed due to increased intensity of competition [Lawes *et al.*, 1882; Lauenroth *et al.*, 1978; Huston, 1997].

The parameterization of the model consisted only in the use of values obtained where the field data were collected, or from the literature about similar sites. The model was not fitted in any manner to the field data. Table 4 presents the values for the biogeochemical parameters used in the simulations for Cedar Creek.

Table 3: Measured Cedar Creek maximum standing biomass [Tilman, 1996].

Year	Nitrogen Addition Rate ($g \cdot m^{-2} \cdot yr^{-1}$)							
	1.0	2.0	3.0	4.4	6.4	10.5	18.0	28.2
1982	150.0	170.0	200.0	200.0	250.0	315.0	425.0	450.0
1983	152.5	175.0	230.0	250.0	315.0	375.0	465.0	530.0
1984	151.5	200.0	230.0	250.0	305.0	380.0	425.0	420.0
1985	151.0	180.0	230.0	234.0	295.0	355.0	415.0	375.0
1986	155.0	200.0	240.0	250.0	365.0	380.0	402.0	360.0
1987	183.5	230.0	255.0	275.0	335.0	338.0	365.0	405.0
1988	89.5	95.0	120.0	118.0	115.0	120.0	125.0	130.0
1989	173.5	185.0	300.0	255.0	255.0	325.0	390.0	330.0
1990	139.5	170.0	190.0	230.0	255.0	255.0	320.0	330.0
1991	184.5	205.0	300.0	250.0	335.0	310.0	375.0	450.0
1992	147.5	178.0	230.0	245.0	275.0	375.0	475.0	580.0
1993	239.0	270.0	350.0	382.0	458.0	445.0	455.0	650.0
1994	168.5	270.0	335.0	245.0	300.0	265.0	365.0	400.0

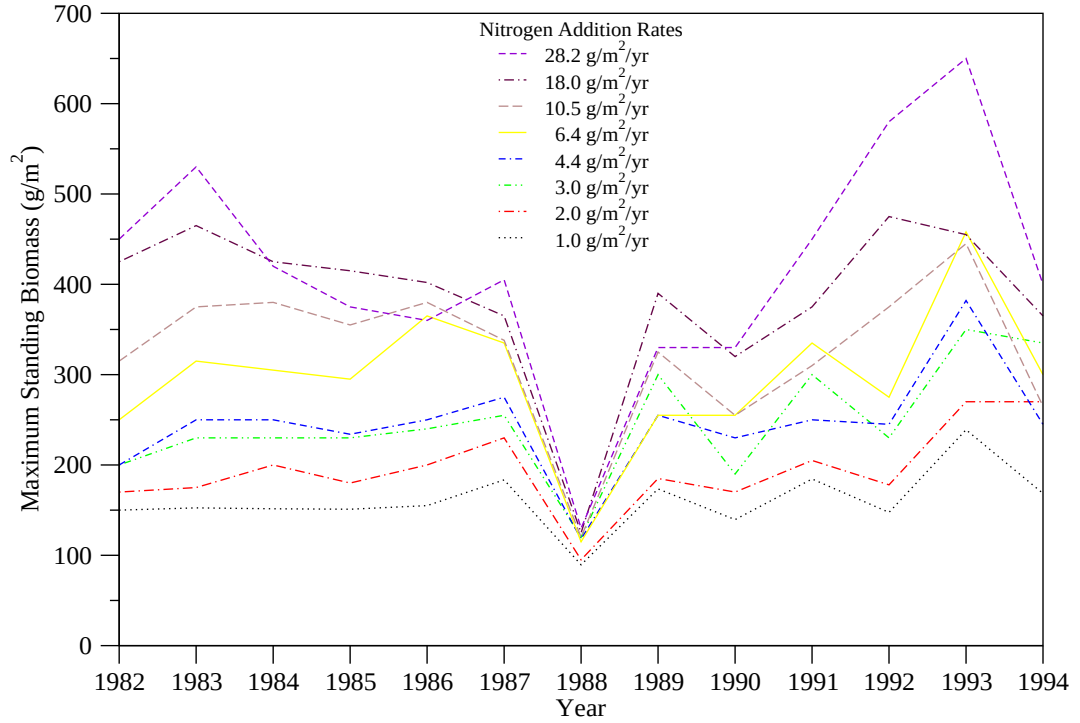


Figure 9: Measured Cedar Creek maximum standing biomass.

Only one grass species with average characteristics was simulated. DNDC allows crop rotation, but not the simultaneous modeling of several plant types.

4.1.2.2 Simulation Results

The simulations consisted of the stand-alone DNDC model in its original and improved versions. The two versions of the lumped model were used to estimate aboveground biomass production for comparison to field data collected at Cedar Creek. Identical input parameters were used for both versions of the model.

Table 5 and Figure 10 show the results of the simulation of the grassland plots with the original version of DNDC. Table 6 and Figure 11 present the results of the same simulation, but with the improved version of DNDC. The original and improved versions of the DNDC model were run for sixteen years. The first three years were “spin-up” years to stabilize the carbon, nitrogen and water pools in the

Table 4: Biogeochemical input parameters for Cedar Creek simulations [from *Hodson, 1985*; *Tilman, 1996*].

Parameter	Value
soil texture	sandy
soil clay fraction	0.03
soil density ($g \cdot cm^{-3}$)	1.50
soil pH	5.5
initial fraction of soil moisture	0.20
initial soil temperature ($^{\circ}C$)	0.0
initial SOC at surface ($kg C \cdot kg^{-1}$)	0.02
initial NO_3^- ($mg N \cdot kg^{-1}$)	0.10
initial NH_4^+ ($mg N \cdot kg^{-1}$)	4.2
initial fraction of passive humus	0.70
initial fraction of litter	0.15
initial fraction of humads	0.15

model. These “spin-up” years utilized normal precipitation and temperature data for the Cedar Creek area and no additional nitrogen besides what occurred naturally in the area.

The model estimates other important biogeochemical properties of the site in addition to aboveground biomass. These include belowground biomass, soil carbon, soil nitrogen, soil and root respiration, nitrogen uptake and leaching, soil C:N ratio, nitrous oxide and nitrogen gas emissions, and actual soil evaporation and plant transpiration. However, none of these parameters were available in the Cedar Creek experiment. Nonetheless, this output from the model was checked for consistency in general trends and amounts against published data from other studies and was found to be in agreement with them.

4.1.3 Distributed Model

4.1.3.1 Measured Data and Input Parameters

The field data collected at the Walker Branch Watershed include measurements of total soil carbon and nitrogen, soil extractable ammonium and nitrate,

Table 5: Simulated Cedar Creek maximum standing biomass, original DNDC.

Year	Nitrogen Addition Rate ($g \cdot m^{-2} \cdot yr^{-1}$)							
	1.0	2.0	3.0	4.4	6.4	10.5	18.0	28.2
1982	202.6	211.8	218.6	225.6	232.4	243.0	259.4	280.8
1983	198.2	210.0	219.8	231.8	246.4	273.2	317.0	365.6
1984	204.8	221.0	234.4	251.2	273.8	323.0	366.6	400.6
1985	203.8	217.4	227.6	239.6	254.6	280.6	322.4	380.0
1986	202.4	219.2	230.8	244.0	260.0	288.2	319.0	354.2
1987	209.2	226.4	236.2	246.6	257.6	272.6	288.4	303.2
1988	198.0	208.6	215.6	223.0	228.4	230.6	233.2	235.2
1989	201.0	218.4	231.0	245.2	263.0	303.8	385.8	423.4
1990	211.8	231.8	244.8	258.8	276.2	301.8	338.8	383.8
1991	208.0	221.4	231.4	242.8	256.8	278.2	308.4	334.0
1992	207.6	224.8	238.6	255.0	276.8	310.0	344.4	372.4
1993	214.4	229.0	240.8	256.0	272.2	298.6	336.8	372.6
1994	208.0	228.4	244.6	257.2	263.4	267.2	270.4	274.4

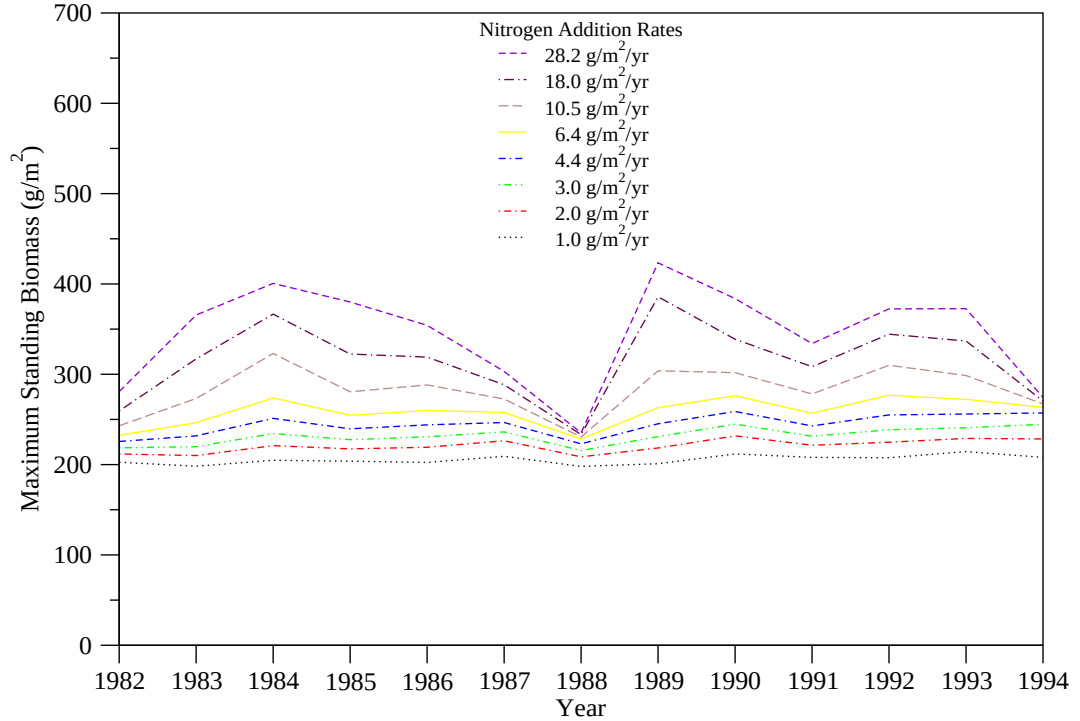


Figure 10: Simulated Cedar Creek maximum standing biomass, original DNDC.

Table 6: Simulated Cedar Creek maximum standing biomass, improved DNDC.

Year	Nitrogen Addition Rate ($g \cdot m^{-2} \cdot yr^{-1}$)							
	1.0	2.0	3.0	4.4	6.4	10.5	18.0	28.2
1982	162.2	221.0	259.2	287.8	312.8	346.8	368.0	421.4
1983	156.0	213.2	249.8	269.0	301.8	365.2	426.6	485.0
1984	159.0	221.8	256.4	295.8	339.8	402.8	471.4	529.8
1985	173.8	241.6	282.2	337.6	378.0	434.8	484.0	535.0
1986	159.0	228.2	271.0	318.0	356.6	401.4	449.4	477.2
1987	130.8	177.4	220.0	253.8	264.8	278.4	296.2	300.2
1988	101.2	121.4	139.2	157.6	172.8	191.6	222.6	261.0
1989	120.6	178.0	205.4	238.2	276.6	311.0	350.6	411.4
1990	136.2	186.6	220.0	252.0	281.6	315.6	366.4	430.0
1991	137.4	195.6	242.8	301.6	354.8	402.8	468.6	547.4
1992	122.6	181.0	224.4	268.8	317.6	364.4	445.8	477.4
1993	135.2	193.8	230.0	280.0	328.0	390.4	475.8	493.0
1994	129.0	190.2	236.2	289.4	331.2	351.2	375.6	383.4

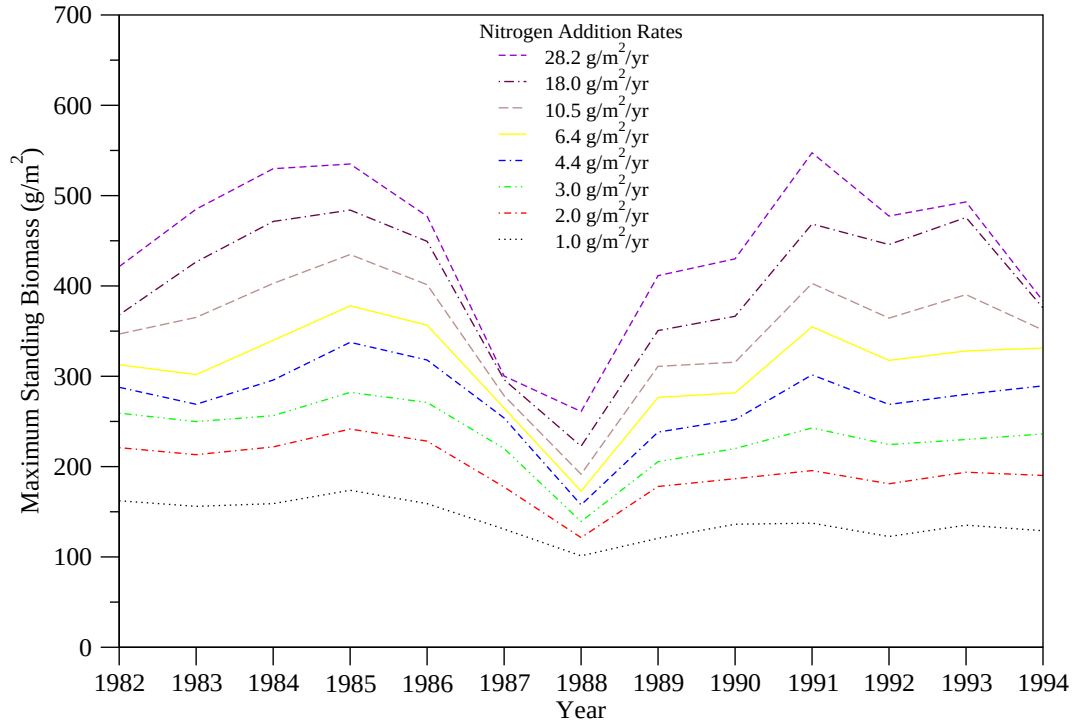


Figure 11: Simulated Cedar Creek maximum standing biomass, improved DNDC.

and nitrification and mineralization rates from laboratory incubations of soil samples. Laboratory incubations are performed under constant and optimal moisture conditions, therefore the nitrification and mineralization rates are not comparable to those simulated by the model under more realistic conditions and will not be used. The field data were gathered by *Garten et al.* [1994] from eighteen sampling stations along transect 6602N, which crosses both subcatchments of the Walker Branch Watershed. This transect had a southwest-northeast orientation with 16 regularly spaced stations and 2 additional stations located in valley floors within 15 m of the stream. Figure 12 shows the location of the transect.

The field data were collected every other month beginning in August, 1989 and ending in August, 1990. Soil data were based on 4 to 8 soil cores (2 cm diameter; 0–7 cm deep) collected within a 10 m radius of each station and composited for subsequent analysis in the laboratory. Samples of deeper soils (7–21 cm deep) were collected for the determination of total soil carbon and nitrogen only. For a detailed

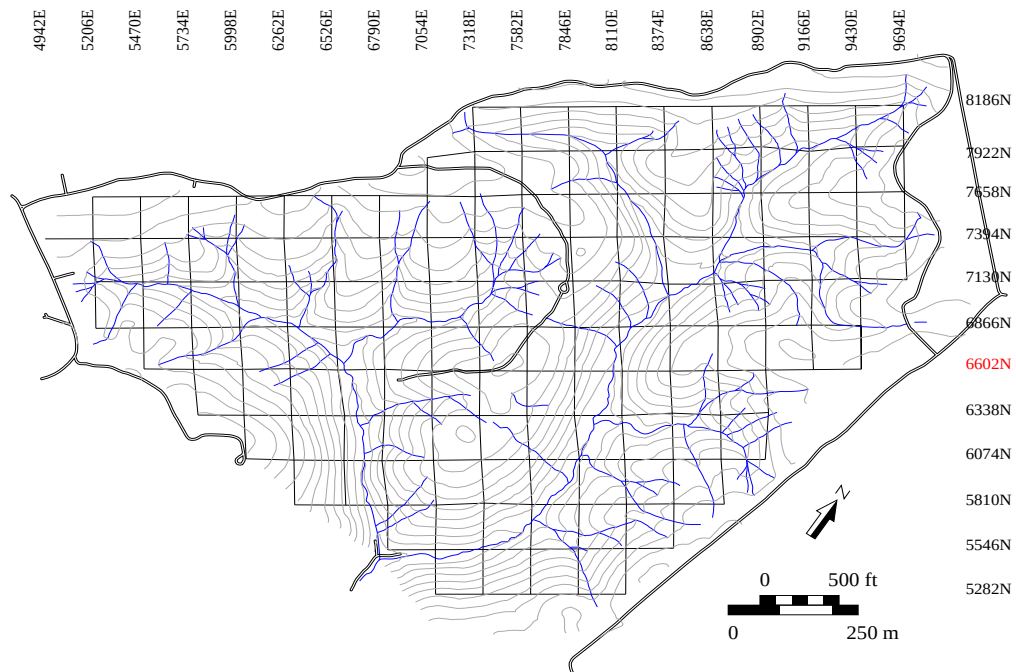


Figure 12: Map of Walker Branch Watershed with transects [Timmins, unpublished].

description of the methods utilized to collect these data, and its analysis, see *Garten et al.* [1994]. It is important to note that the work of *Garten et al.* [1994] found statistically significant differences in soil properties with respect to topographic location (ridge, valley, and slope) within a watershed, as well as significant correlations between the topographic index ($a/\tan\beta$) and various soil properties.

Table 7 presents the field data values for the extractable soil ammonium and nitrate at each of the transect stations in the Walker Branch Watershed. The stations in the table are characterized according to their topographic position (ridge, valley, and slope). The field data were averaged into four seasons for simplicity and also because the data show strong seasonal variations.

Table 8 shows the field data values for the total soil nitrogen and carbon, and the soil carbon to nitrogen ratio. These data are not expected to vary much with time, and were not collected seasonally. Any variations in their values may only indicate error in sample location, methods, or analysis. Hence, the values presented in Table 8 are averages of two separate collections.

As in the Cedar Creek case, the parameterization of the biogeochemical component of TOPDNDC consisted only of the use of values obtained where the field data were collected, or from the literature concerning similar sites. No biogeochemical parameters were fitted to the field data. Table 9 presents the main biogeochemical parameters utilized by TOPDNDC for the Walker Branch simulations. The Walker Branch Watershed receives approximately $1.4 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$ of nitrogen via natural atmospheric deposition [*Lindberg et al.*, 1989]. This level of nitrogen was augmented to $2.0 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$ to compensate for the lack of nitrogen-fixing species in the model, which increase the amount of nitrogen available in the soil.

Although field data were available for the entire Walker Branch Watershed, this study modeled and compared only the West Fork Catchment of the watershed (see Section 3.1.3 for a description of Walker Branch Watershed). The entire wa-

Table 7: Measured Walker Branch Watershed soil extractable ammonium and nitrate, (0 – 7 cm) [*Garten et al.*, 1994].

Station	Site	Elev. (m)	$a/\tan\beta$	$\text{NH}_4^+ (gN \cdot m^{-2})$			$\text{NO}_3^- (gN \cdot m^{-2})$				
				Spring	Summer	Fall	Winter	Spring	Summer	Fall	Winter
E5470	ridge	334	5.64	0.42	0.22	0.16	0.53	0.002	0.091	0.058	0.004
E5734	slope	328	6.29	0.29	0.18	0.09	0.39	0.001	0.083	0.144	0.003
E5998	slope	317	7.52	0.48	0.20	0.30	0.74	0.000	0.050	0.059	0.003
E6262	slope	306	7.10	0.47	0.31	0.41	1.05	0.000	0.028	0.051	0.004
E6526	slope	287	6.73	0.39	0.25	0.21	0.89	0.000	0.026	0.068	0.004
E6624	valley	282	12.00	0.80	0.43	0.63	1.44	0.000	0.118	0.071	0.005
E6790	slope	299	6.34	0.13	0.05	0.13	0.35	0.006	0.021	0.000	0.002
E7054	slope	317	5.25	0.21	0.09	0.07	0.26	0.000	0.053	0.034	0.001
E7318	slope	328	5.45	0.21	0.10	0.17	0.45	0.000	0.020	0.037	0.001
E7582	slope	326	5.84	0.45	0.20	0.31	1.00	0.000	0.023	0.060	0.003
E7846	slope	305	6.30	0.23	0.17	0.19	0.87	0.000	0.012	0.081	0.002
E8044	valley	285	15.00	1.01	0.61	0.76	2.32	0.040	0.072	0.126	0.023
E8110	slope	293	5.99	0.10	0.10	0.09	0.38	0.000	0.049	0.040	0.002
E8374	ridge	323	5.18	0.20	0.09	0.12	0.28	0.000	0.009	0.053	0.005
E8638	slope	323	5.47	0.27	0.16	0.29	0.48	0.000	0.011	0.031	0.004
E8902	slope	334	6.63	0.43	0.24	0.30	0.72	0.003	0.023	0.050	0.003
E9166	ridge	340	6.50	0.24	0.17	0.13	0.50	0.000	0.010	0.000	0.001
E9430	ridge	341	5.88	0.24	0.11	0.12	0.50	0.003	0.030	0.048	0.002

Table 8: Measured Walker Branch Watershed total soil carbon, nitrogen, and C:N ratio at two different depths [*Garten et al.*, 1994].

Station	Site	Elev. (m)	$a/\tan\beta$	0 – 7 cm				7 – 21 cm			
				Soil N (%)	Soil N ($gN \cdot m^{-2}$)	Soil C (%)	Soil C ($gC \cdot m^{-2}$)	Soil C:N	Soil N (%)	Soil C (%)	Soil C:N
E5470	ridge	334	5.64	0.09	97.44	2.39	2506.35	26.11	0.06	1.24	22.07
E5734	slope	328	6.29	0.15	162.54	2.88	3024.32	18.40	0.07	1.44	20.33
E5998	slope	317	7.52	0.16	171.36	2.83	2971.87	17.46	0.07	0.72	10.80
E6262	slope	306	7.10	0.15	155.98	2.11	2220.12	14.22	0.06	0.67	11.07
E6526	slope	287	6.73	0.18	191.73	3.09	3249.59	16.98	0.08	0.98	11.97
E6624	valley	282	12.00	0.25	263.76	3.95	4148.55	15.74	0.11	1.63	15.21
E6790	slope	299	6.34	0.12	123.38	2.53	2656.82	21.50	0.07	1.00	14.11
E7054	slope	317	5.25	0.09	93.56	1.73	1818.18	20.39	0.03	0.41	15.10
E7318	slope	328	5.45	0.15	158.50	3.78	3968.11	23.23	0.14	2.48	17.47
E7582	slope	326	5.84	0.19	195.20	3.78	3971.68	20.14	0.06	1.11	19.29
E7846	slope	305	6.30	0.14	145.95	2.52	2648.05	17.91	0.04	0.64	14.67
E8044	valley	285	15.00	0.23	243.97	3.14	3299.00	13.55	0.09	0.77	8.98
E8110	slope	293	5.99	0.11	118.60	2.79	2929.19	24.72	0.04	0.54	14.24
E8374	ridge	323	5.18	0.10	110.20	2.79	2927.45	26.57	0.05	0.91	19.25
E8638	slope	323	5.47	0.15	153.98	3.19	3351.55	21.74	0.04	0.97	22.21
E8902	slope	334	6.63	0.14	143.80	2.94	3092.15	21.50	0.08	0.84	11.15
E9166	ridge	340	6.50	0.13	137.18	2.63	2760.14	20.12	0.04	0.64	14.87
E9430	ridge	341	5.88	0.13	133.56	2.42	2536.96	19.06	0.04	0.40	9.07

tershed is underlain by bedrock consisting of highly fractured dolomite of the Knox Group. However, only the East Fork of the Walker Branch Watershed shows typical karstic behavior of intermittent flow in reaches [*Huston and Fontaine, 1994*]. The West Fork has a small, relatively constant inflow from outside the catchment boundary, but it has been well characterized and can be modeled as an inflow independent of local precipitation and hydrologic conditions [*Luxmoore and Huff, 1989*]. Most hydrologic research and modeling have focused on the West Fork.

The hydrological component of TOPDNDC requires the use of hourly precipitation records. The hourly precipitation records available for Walker Branch Watershed encompass the years 1985-1996, and the years 1999 and 2000. However, this period of record includes one of the worst droughts of the past 100 years in East Tennessee. The drought lasted from 1985 until 1988 as can be seen in Figure 13, which shows the Palmer Drought Severity Index (PDSI) for East Tennessee (NCDC Climate Division 1) in the last 30 years.

The simulations carried out in TOPDNDC for comparison with field data involved long term soil parameters that accumulate and stabilize through time.

Table 9: Biogeochemical input parameters for Walker Branch Watershed simulations [from *Johnson, 1989; Stange et al., 2000*].

Parameter	Value
soil texture	silt loam
soil clay fraction	0.14
soil density ($g \cdot cm^{-3}$)	1.50
soil pH	4.8
initial fraction of soil moisture	0.40
initial soil temperature ($^{\circ}C$)	10.0
initial SOC at surface ($kgC \cdot kg^{-1}$)	0.025
initial NO_3^- ($mgN \cdot kg^{-1}$)	0.02
initial NH_4^+ ($mgN \cdot kg^{-1}$)	5.20
initial fraction of passive humus	0.40
initial fraction of litter	0.36
initial fraction of humads	0.24

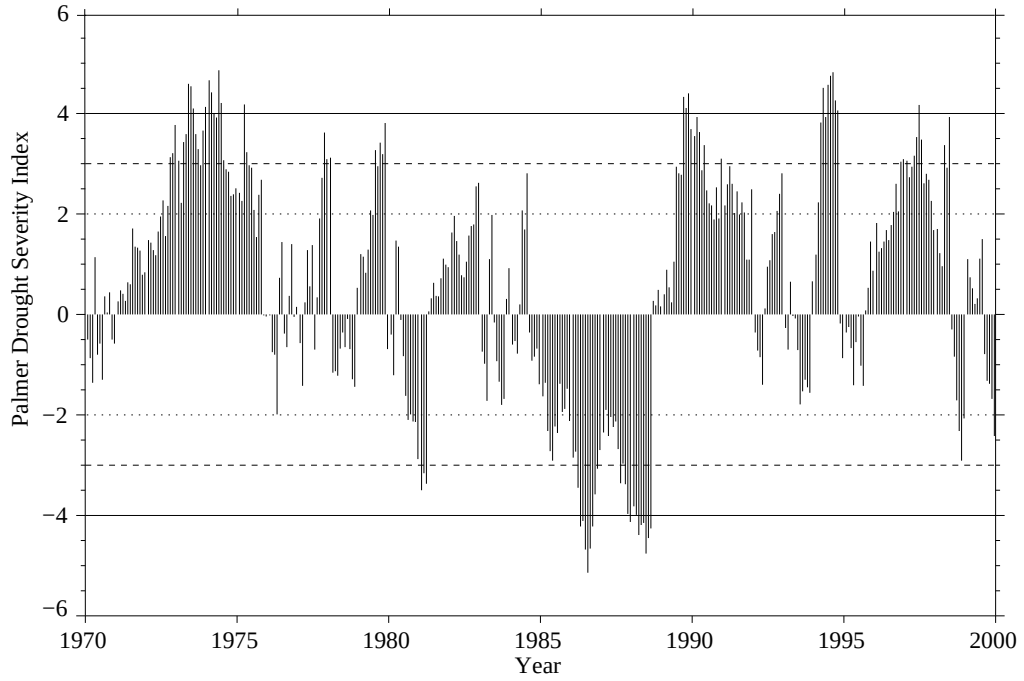


Figure 13: East Tennessee Palmer Drought Severity Index.

Therefore, starting the simulation with an extreme drought would not allow the model to simulate these parameters properly. Instead, a synthetic “normal” time series was created using only precipitation data from 1989 until 1996, and 1999 and 2000 and repeated as needed to cover a long term period, in this case, 13 years, which includes three years of model “spin-up”.

The hydrological component of TOPDNDC utilized the same calibration parameters of *Huston and Fontaine* [1994], who found that TOPMODEL accurately predicted the flood hydrograph and the extent of overland flow on the West Fork of the Walker Branch Watershed when properly calibrated.

TOPDNDC required the calculation of the distribution of topographic index in the catchment to classify the varying “wetness” of the areas where biogeochemical processes occur. For this study, the topographic index was divided into 10 classes. Other studies have categorized the topographic index in up to 65 classes. However, the trade off between computational speed and the needed spatial resolution did not

warrant the use of more than 10 classes. Increasing the number of classes would increase the computational time of TOPDNDC since the biogeochemical component of TOPDNDC runs once each day for every topographic class (see Section 3.4).

Figure 14 shows the DEM of the West Fork of the Walker Branch Watershed with the topographic index map superimposed on it. Dark blue represents areas like valleys and stream channels that have a high potential for development of water saturation, white colors areas like ridges that have low saturation potential, the different shades of blue show the potential degree of water saturation between the high and low extremes. The DEM had a cell resolution of 10 x 10 ft (3 x 3 m) and was derived from a contour map with 2 ft (0.61 m) contour intervals [*Timmins et al.*, 1989].

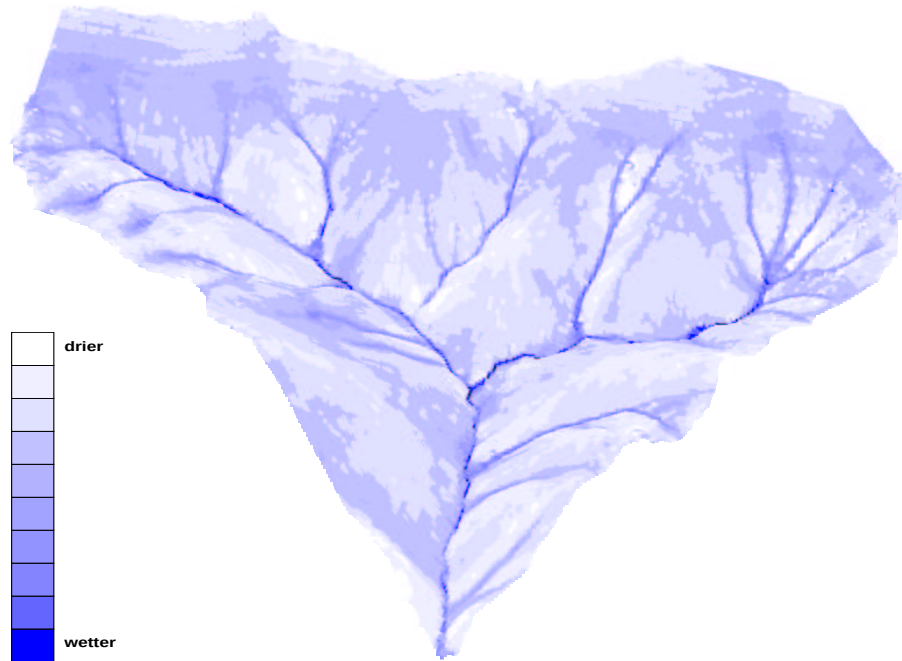


Figure 14: DEM and topographic index classes for the West Fork Catchment of the Walker Branch Watershed.

4.1.3.2 Simulation Results

Two different simulations of the biogeochemical processes taking place on the West Fork of the Walker Branch Watershed were performed with TOPDNDC. The first simulation modeled the entire West Fork Catchment with only one type of forest. It was executed to look at patterns of change in soil carbon and nitrogen, and forest growth across the watershed solely due to variations in soil moisture. The second simulation involved the parameterization of different forest types according to their location on the Walker Branch Watershed. TOPDNDC was not designed to perform forest succession, which occurs over several hundreds of years of simulation. However, by having different types of forests on the catchment the result of forest succession on the biogeochemical processes can be simulated.

The distribution of forest types in the Walker Branch Watershed follows soil moisture patterns. Tulip poplar and beech forests are located near the stream, which is the wettest area of the catchment, one that has a high topographic index. Pine forests grow on the ridges, the driest location in the catchment, which has a very low topographic index. Oak and hickory forests mostly dominate the slopes that have intermediate values of wetness and topographic indices.

Different forest types vary in potential relative growth rate, LAI, height, leaf, trunk and root C:N ratios and root:leaf:trunk proportion, all of which are in TOPDNDC. For the second simulation presented here the only parameters modified to differentiate between forest types were the optimum leaf C:N ratio and the potential relative growth rate.

The leaf C:N ratio in TOPDNDC has a double influence in tree growth (see Section 3.2.3). First, it limits the maximum tree growth as the model restricts carbon uptake if there is not enough nitrogen available. Secondly, it influences tree growth after leaf fall by returning the nitrogen in the dead leaves to the soil. The potential relative growth rate is tightly linked to leaf C:N ratio in the model through

the plant growth equation (see Equation 31). Limiting the parameter variation to these two properties allows the evaluation of their effects in different types of forests on different parts of the landscape without introducing changes in other parameters that may or may not have a significant effect on the biogeochemistry of forest growth.

Table 10 presents the optimum live leaf C:N ratio and the potential relative growth rate for the different forest types used in the second simulation of the West Fork of the Walker Branch Watershed with TOPDNDC.

Table 11 presents the average of the last three years of the TOPDNDC simulation for total soil carbon and nitrogen at two depths with the same type of forest covering the whole West Fork of the Walker Branch Watershed. There is not an exact match between the depth of the soil collected in the field and the depth modeled. TOPDNDC simulates soil behavior by dividing the soil profile into discrete layers of fixed depth. The layer in the model presented in the table is the closest to the one in the field. Table 12 shows the same results as the previous table but for a forest composed of different types of trees.

Table 13 presents the seasonal average of the last three years of the model simulation for the total soil ammonium and nitrate at 7.5 cm assuming only one forest type covers the entire watershed. Table 14 shows the same results as the previous table, but with different types of forests covering the watershed.

Table 10: TOPDNDC simulation, optimum C:N ratio of live forest leaves and potential relative growth rate [from *Grizzard et al., 1976*].

Forest	Site	Leaf N (%)	Leaf C (%)	Leaf C:N	Growth Rate
shortleaf pine	ridge	1.7	50	29	0.05
oak	slope	2.2	50	23	0.06
hickory	slope	2.4	50	21	0.07
beech	valley	2.6	50	19	0.09
tulip poplar	valley	2.8	50	18	0.10

Table 11: Simulated Walker Branch Watershed average of last three years of soil carbon, nitrogen, and C:N ratio at two different depths, one forest type TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	0 – 7.5 cm			7.5 – 20 cm		
			Soil N (%)	Soil N ($gN \cdot m^{-2}$)	Soil C (%)	Soil N (%)	Soil C (%)	Soil C:N
ridge	4.74	1	0.268	296.19	4.41	0.06	0.86	13.75
ridge	5.62	2	0.268	295.89	4.41	0.06	0.85	13.75
slope	6.45	3	0.268	295.43	4.41	0.06	0.85	13.76
slope	7.36	4	0.267	294.86	4.41	0.06	0.85	13.77
slope	8.41	5	0.266	293.89	4.41	0.06	0.85	13.82
slope	9.47	6	0.267	294.63	4.41	0.06	0.85	13.80
slope	10.46	7	0.268	295.66	4.41	0.06	0.84	13.72
slope	11.46	8	0.269	296.76	4.39	0.06	0.85	13.69
valley	12.45	9	0.270	298.16	4.38	0.06	0.85	13.64
valley	13.98	10	0.273	301.09	4.35	0.06	0.84	13.49

Table 12: Simulated Walker Branch Watershed average of last three years of soil carbon, nitrogen, and C:N ratio at two different depths, several forest types TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	0 – 7.5 cm				7.5 – 20 cm			
			Soil N (%)	Soil N ($gN \cdot m^{-2}$)	Soil C (%)	Soil C ($gC \cdot m^{-2}$)	Soil N (%)	Soil N (%)	Soil C (%)	Soil C (%)
ridge	4.74	1	0.260	286.89	4.51	4979.03	0.06	0.06	0.85	14.21
ridge	5.62	2	0.260	286.52	4.51	4973.73	0.06	0.06	0.85	14.21
slope	6.45	3	0.267	295.13	4.41	4866.50	0.06	0.06	0.85	13.77
slope	7.36	4	0.267	294.86	4.41	4864.57	0.06	0.06	0.85	13.77
slope	8.41	5	0.267	294.13	4.41	4863.13	0.06	0.06	0.85	13.79
slope	9.47	6	0.267	295.23	4.40	4858.80	0.06	0.06	0.85	13.76
slope	10.46	7	0.268	296.09	4.40	4853.07	0.06	0.06	0.84	13.72
slope	11.46	8	0.270	297.66	4.39	4841.10	0.06	0.06	0.85	13.66
valley	12.45	9	0.271	299.16	4.37	4824.27	0.06	0.06	0.84	13.58
valley	13.98	10	0.274	302.86	4.33	4780.30	0.06	0.06	0.85	13.40

Table 13: Simulated Walker Branch Watershed seasonal average of last three years of soil ammonium and nitrate, one forest type TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	$\text{NH}_4^+ (gN \cdot m^{-2})$			$\text{NO}_3^- (gN \cdot m^{-2})$		
			Spring	Summer	Fall	Spring	Summer	Fall
ridge	4.74	1	0.263	0.183	0.203	0.014	0.005	0.005
ridge	5.62	2	0.263	0.187	0.203	0.015	0.005	0.005
slope	6.45	3	0.260	0.187	0.203	0.015	0.005	0.005
slope	7.36	4	0.260	0.187	0.200	0.015	0.005	0.005
slope	8.41	5	0.260	0.190	0.200	0.015	0.006	0.005
slope	9.47	6	0.260	0.190	0.200	0.015	0.006	0.005
slope	10.46	7	0.260	0.210	0.203	0.015	0.006	0.005
slope	11.46	8	0.260	0.210	0.203	0.015	0.006	0.005
valley	12.45	9	0.260	0.213	0.207	0.015	0.006	0.006
valley	13.98	10	0.267	0.213	0.217	0.016	0.007	0.006

Table 14: Simulated Walker Branch Watershed seasonal average of last three years of soil ammonium and nitrate, several forest types TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	$\text{NH}_4^+ (gN \cdot m^{-2})$			$\text{NO}_3^- (gN \cdot m^{-2})$		
			Spring	Summer	Fall	Spring	Summer	Fall
ridge	4.74	1	0.253	0.180	0.190	0.193	0.005	0.005
ridge	5.62	2	0.253	0.183	0.190	0.193	0.005	0.005
slope	6.45	3	0.260	0.187	0.200	0.203	0.005	0.005
slope	7.36	4	0.260	0.187	0.200	0.203	0.005	0.005
slope	8.41	5	0.260	0.190	0.200	0.200	0.006	0.005
slope	9.47	6	0.260	0.190	0.200	0.203	0.006	0.005
slope	10.46	7	0.260	0.210	0.203	0.203	0.006	0.005
slope	11.46	8	0.260	0.210	0.203	0.207	0.006	0.005
valley	12.45	9	0.263	0.213	0.210	0.207	0.006	0.006
valley	13.98	10	0.267	0.213	0.223	0.210	0.007	0.006

Table 15: Simulated Walker Branch Watershed total annual live trunk biomass, one forest type TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	Trunk Biomass ($g \cdot m^{-2}$)												
			1	2	3	4	5	6	7	8	9	10	11	12	13
ridge	4.74	1	11496	11312	11247	11069	11218	11058	11928	12948	12703	12510	12997	12966	12770
ridge	5.62	2	11518	11337	11343	11167	11385	11224	12111	13152	12904	12710	13256	13275	13094
slope	6.45	3	11565	11386	11438	11263	11545	11385	12376	13425	13172	12976	13650	13723	13558
slope	7.36	4	11581	11403	11501	11328	11743	11590	12592	13673	13415	13220	14048	14149	14057
slope	8.41	5	11621	11446	11605	11434	12131	12058	13094	14165	13899	13697	14596	14713	14690
slope	9.47	6	11637	11462	11692	11522	12298	12273	13311	14442	14171	13967	15001	15210	15235
slope	10.46	7	11663	11491	11789	11620	12429	12485	13538	14724	14449	14243	15419	15739	15845
slope	11.46	8	11711	11541	11938	11770	12708	12749	13830	15058	14777	14570	15903	16252	16482
valley	12.45	9	11738	11570	12031	11864	12884	12941	14042	15355	15069	14862	16299	16642	16913
valley	13.98	10	11766	11600	12126	11992	13055	13223	14316	15642	15353	15144	16724	17178	17460

Table 16: Simulated Walker Branch Watershed total annual live trunk biomass, several forest types TOPDNDC.

Site	$a/\tan\beta$	$a/\tan\beta$ Class	Trunk Biomass ($g \cdot m^{-2}$)												
			Year												
			1	2	3	4	5	6	7	8	9	10	11	12	13
ridge	4.74	1	11683	11501	12072	11885	12433	12256	13183	14177	13909	13697	14079	14030	13818
ridge	5.62	2	11735	11556	12137	11952	12608	12452	13396	14399	14127	13913	14368	14393	14177
slope	6.45	3	11619	11439	11565	11388	11542	11381	12342	13369	13117	12920	13407	13424	13226
slope	7.36	4	11635	11458	11641	11465	11718	11566	12538	13596	13339	13144	13727	13779	13619
slope	8.41	5	11648	11473	11755	11580	11999	11905	12914	13966	13703	13504	14217	14313	14226
slope	9.47	6	11637	11462	11703	11533	12260	12192	13201	14310	14041	13838	14772	14940	14917
slope	10.46	7	11663	11491	11817	11647	12455	12451	13505	14661	14386	14182	15231	15449	15495
slope	11.46	8	11711	11541	11938	11769	12583	12657	13707	14921	14643	14437	15575	15885	15980
valley	12.45	9	11712	11543	11916	11750	12773	12855	13957	15273	14989	14784	16223	16644	16890
valley	13.98	10	11711	11545	11909	11758	12827	12977	14111	15483	15198	14992	16643	17099	17395

Table 15 and Table 16 show the total annual live trunk biomass during the 13 years of simulation for forests composed of one type and several types of trees respectively. Most of the annual variation in aboveground biomass is due to trunk production. Tree leaves come out rapidly in spring, reaching a constant biomass that may vary only under severe environmental conditions, like extreme drought.

4.2 Discussion of Results

4.2.1 Introduction

The discussion of results is divided into two sections. The first section includes comments on the results of the lumped model (stand-alone DNDC) for Cedar Creek. The second section discusses the results obtained by the distributed model TOPDNDC for Walker Branch.

4.2.2 Lumped Model

Figure 15 presents a graphical comparison between the field data and the two DNDC model versions for all levels of nitrogen addition. In general, the results of the improved DNDC version followed more closely the field data obtained at Cedar Creek. The original DNDC formulation was not able to produce any temporal variations in aboveground biomass except for high levels of nitrogen (18.0 and $28.2 \text{ g N} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$). It seems that the original DNDC version is capable of simulating only the mean behavior of the data, whereas the new version is also capable of reproducing a large proportion of the temporal and treatment variability in the data.

The correlation coefficient (r) for both versions of the model was calculated using all data points, regardless of the nitrogen addition. The original version of the model had a correlation coefficient of 0.79 with respect to the maximum standing biomass measured at Cedar Creek. The improved version of the model had a higher correlation of 0.85 . Figure 16 illustrates the relationship between the measured and

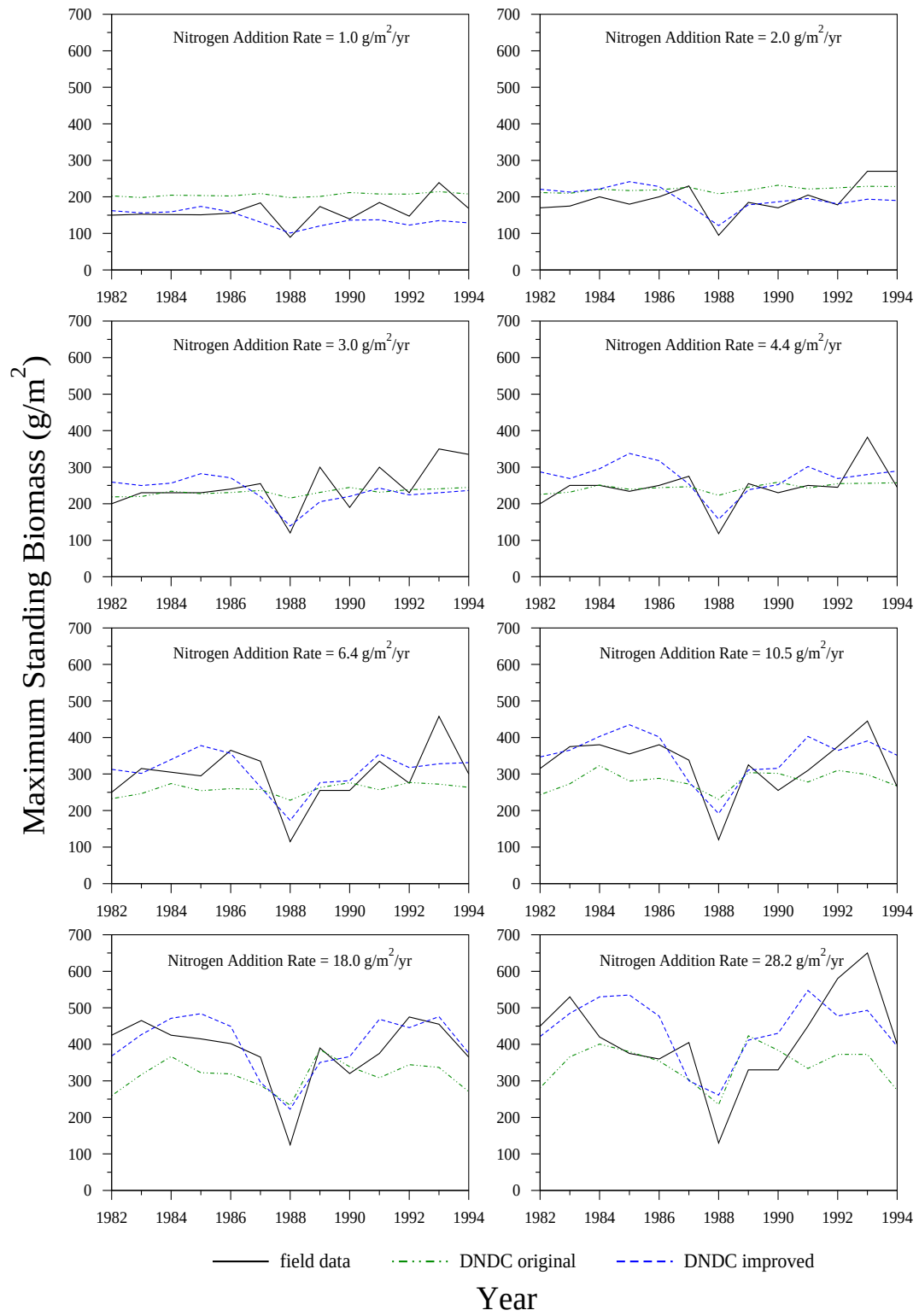


Figure 15: Cedar Creek comparison matrix of field data and models simulations.

simulated values of aboveground biomass for Cedar Creek. The improved version of the model fitted the measured data better than the original version, and it also had a wider spread in the values than the original model (more variability). Both regression lines in Figure 16 were statistically significant with p-values of less than 0.01. The regression line for the original version of the model was defined by $y = 0.37 \cdot x + 1.57.83$ and had an adjusted r^2 of 0.62. The improved version regression line was $y = 0.84 \cdot x + 55.60$ with an adjusted r^2 of 0.71.

Model comparison should ideally include a quantitative statistical appraisal besides the typical visual/graphical assessment. Table 17 presents this statistical comparison of the original and improved DNDC models against the field data collected at Cedar Creek.

The indicators used for the quantitative evaluation are the root mean square error (RMSE), the modeling efficiency (EF), the coefficient of determination (CD),

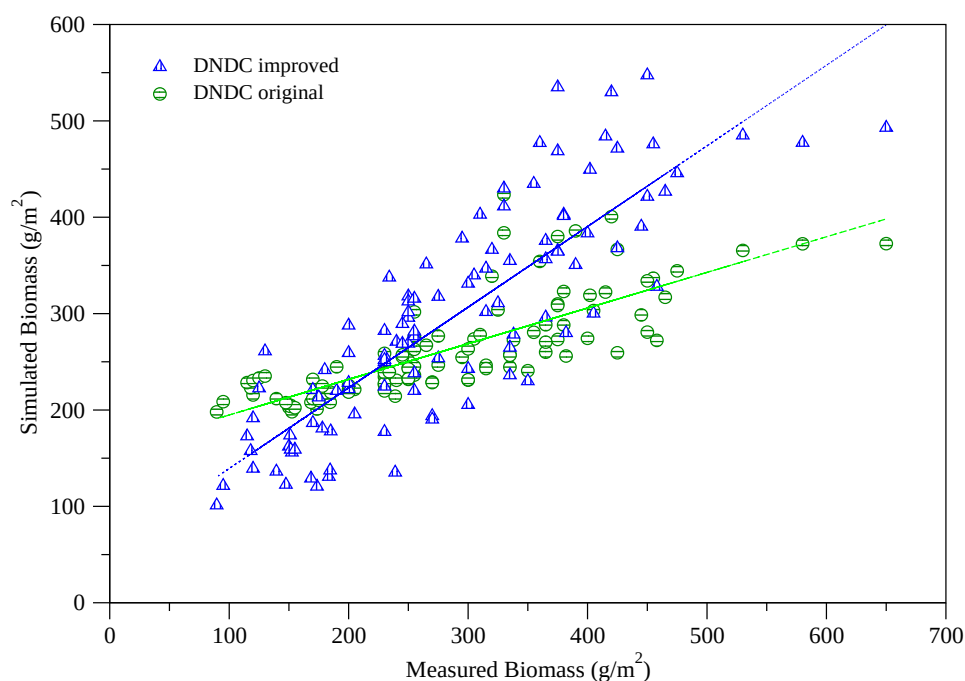


Figure 16: Cedar Creek measured vs simulated values for the two versions of DNDC model.

Table 17: Cedar Creek quantitative evaluation of DNDC models against field data.

Nitrogen Addition ($g \cdot m^{-2} \cdot yr^{-1}$)	RMSE		EF		CD		CRM	
	original	improved	original	improved	original	improved	original	improved
1.0	33.469	25.438	-1.771	-0.600	0.509	1.307	-0.280	0.126
2.0	24.248	22.634	-0.161	-0.012	2.602	2.197	-0.134	-0.009
3.0	23.208	24.399	0.088	-0.008	11.604	2.634	0.061	0.054
4.4	19.610	23.730	0.218	-0.144	22.979	1.138	0.002	-0.115
6.4	26.431	19.110	-0.093	0.427	3.353	2.073	0.129	-0.041
10.5	23.849	17.044	-0.016	0.481	2.347	1.329	0.134	-0.075
18.0	26.046	14.774	-0.352	0.565	1.121	1.232	0.182	-0.040
28.2	32.542	25.285	-0.199	0.276	1.920	1.964	0.172	-0.063

and the coefficient of residual mass (CRM). These indicators are widely used for comparing models by the soil and hydrological sciences [*Loague and Green, 1991; Smith et al., 1997; Vanclooster et al., 2000*].

RMSE measures the total difference between all pairs of the simulated and measured values. A lower RMSE value indicates a smaller difference. EF provides a comparison of the efficiency of the chosen model to the efficiency of describing the data as the mean of the observations. A positive value indicates that the simulated values describe the trend in the measured data better than the mean of the observations. A negative value indicates that the simulated values describe the data less well than a mean of the observations. CD is a measure of the proportion of the total variance in the measured data that is explained by the simulated data. The lower limit for CD is 0, in which case the measured values do not deviate from the mean, and therefore this statistic can provide no information about the variance. A CD value above 1 indicates that the deviation of the simulated values from the mean of the measured ones is less than that observed in the measurements. A CD of less than 1 indicates that the deviation of the simulated values from the mean of the measured values is greater than that observed in the measurements. A CD value of 1 denotes no difference between the variances in the measured and simulated values. CRM gives an indication of the consistency of the errors in the distribution of all simulated values across all measurements with no consideration of the order of the measurements. A negative value indicates that the majority of simulated values are greater than the measured values; a positive value indicates that the majority of the simulated values are less than the measured values.

From the statistical indicators in Table 17, it can be seen that the improved version of the model was better in describing the general pattern of the Cedar Creek field data. The original version had a good fit to the measured data only with an average nitrogen addition, whereas the improved version had a better fit for the

extremes and overall. The improved model had a lower RMSE and a smaller CRM (closer to zero) than the original model for most of the cases. The improved model CD was slightly above 1 for all nitrogen additions, and positive in EF for the second half of the cases. The EF of the original model was negative for all, except two nitrogen additions and also had a CD below 1 and two CD values much greater than one. The CD less than 1 indicated that the original model greatly overpredicted in one instance. The CD values much greater than 1 meant that the original model also greatly underpredicted in two other instances.

Even if the improved DNDC version had merely equaled, and not out performed the original formulation of DNDC, it would constitute an improvement. The plant growth routine of the improved model is mechanistic. Unlike the original DNDC formulation, the improved DNDC does not estimate plant growth based on a time dependent optimal growth curve driven by the elapsed fraction of the growing season (see Section 3.2.2), but rather uses a mechanistic function of interacting growth factors (see Section 3.2.3).

Water and nitrogen were the two main factors controlling the patterns in Figure 15. Both parameters limit the growth of plants; nitrogen by being a required element for chlorophyll, photosynthesis, and growth, water by making this nutrient available to the plant roots for uptake and through transpiration.

The most obvious effect of water on plant growth can be seen during the peak of the drought in 1988. In all cases, the plant biomass (plant growth) was reduced drastically during this year, regardless of the level of nitrogen addition. The model was able to reproduce this water limiting effect successfully, except for the large nitrogen addition cases (18.0 , and $28.2 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$), where the drop in plant biomass is not as pronounced as it is in the field data. The model allows moderate plant growth to occur during a drought when large amounts of nitrogen are added. Since the model does not limit the concentration of nitrogen dissolved in

the soil water, as long as there is water in the soil above the wilting point, nutrients (nitrogen) are absorbed by the roots. This is not the case in nature, where the large amount of nitrogen may be toxic to the plant and not absorbed. Another plausible explanation would be that physiologically, plants are more efficient at absorbing low levels of nitrogen than high levels. It is important to note that these high levels of nitrogen addition are over nine times those found in undisturbed grasslands.

At the lowest level of nitrogen addition ($1.0 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$) the model did not perform very well. The apparent lack of fit may be explained by the low level of nitrogen itself. A nitrogen addition of $1.0 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$ represents the natural atmospheric deposition of nitrogen for the Cedar Creek area. However, legumes grow in grasslands, fixing nitrogen from the air and increasing the amount of nitrogen available in the soil. The model does not account for the increased soil nitrogen due to the presence of legumes, and therefore the model nitrogen input for this case is lower than the unfertilized plot.

At medium levels of nitrogen addition (2.0, 3.0, 4.4, 6.4, and $10.5 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$), the model performed better, matching more closely the observed productivity, including the drop in aboveground biomass during the 1988 drought. However, it was not able to reproduce the rapid increase in biomass production between 1992 and 1993 and tended to overpredict during the first years of the simulation. The increased production during the first years of simulation may be due to high starting rates of mineralization of soil organic matter in the model. Microbes in the model decompose organic nitrogen, generating inorganic nitrogen that can be utilized by the plants to grow. This process may be occurring at higher rates in the model than in the actual grassland. Additional years of “spin-up” in the model may be required to stabilize the organic matter and microbe pools to levels closer to the ones found in the grassland. Modifying the decomposition parameters in the model may also

improve the simulation during the first years. However, decomposition parameter data are difficult to obtain and validate for use in the model.

The lack of a positive biomass response of the model in 1993 is more difficult to explain. The year 1993 was a wet year in Cedar Creek, and grassland productivity is greatly affected by precipitation [*Knapp and Smith, 2001*]. However, it was also a cool growing season, which may have delayed and reduced the translocation of resources from the roots to the leaves at the beginning of the growing season. The model was not able to overcome this slow and reduced starting condition even with higher than normal precipitation.

With large nitrogen additions (18.0 , and $28.2 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$), the model simulates a system that is no longer nitrogen limited, but instead is water limited. The model showed a better performance for a nitrogen addition of $18 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$ than for $28.2 \text{ g} \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$. At the highest level of nitrogen addition, the model was not able to simulate the large biomass production of the years 1992 and 1993. This may be due to the water use efficiency parameter utilized in the model (see Section 3.2.3), which limits the amount of plant growth at large transpiration rates.

4.2.3 Distributed Model

The distribution of moisture in the catchment allowed the simulation of biomass production and soil nutrient availability on a temporal and spatial scale.

Figure 17 presents a graphical comparison of the total soil nitrogen with respect to its topographic position for the two simulations performed at the West Fork Catchment. Each bar set goes from the total soil nitrogen value for a low topographic index (ridge) to the nitrogen value for a high topographic index (valley). Both simulations showed the same pattern as the measured data, though the simulation using several forest types displayed it more clearly. The increased total nitrogen

in wetter areas (high topographic index) was due to the higher plant uptake and, therefore, less leaching in the presence of water.

Figure 18 presents the comparison of the measured and simulated values of total soil carbon at the West Fork Catchment. There was no apparent trend in the measured data of total soil carbon with respect to the topographic index. The simulated data showed a slight downward trend in the soil carbon from low topographic index to high topographic index sites. Total soil carbon does not vary much with respect to time, and since the period of simulation was only 13 years, the soil carbon pools in the model have probably not reached equilibrium yet. However, the lower total soil carbon on the wetter sites (high topographic index) in the model was probably due to the higher decomposition rates existing in wetter areas.

The measured and simulated numerical values for the total soil nitrogen and carbon were significantly different. The total soil nitrogen in the model output

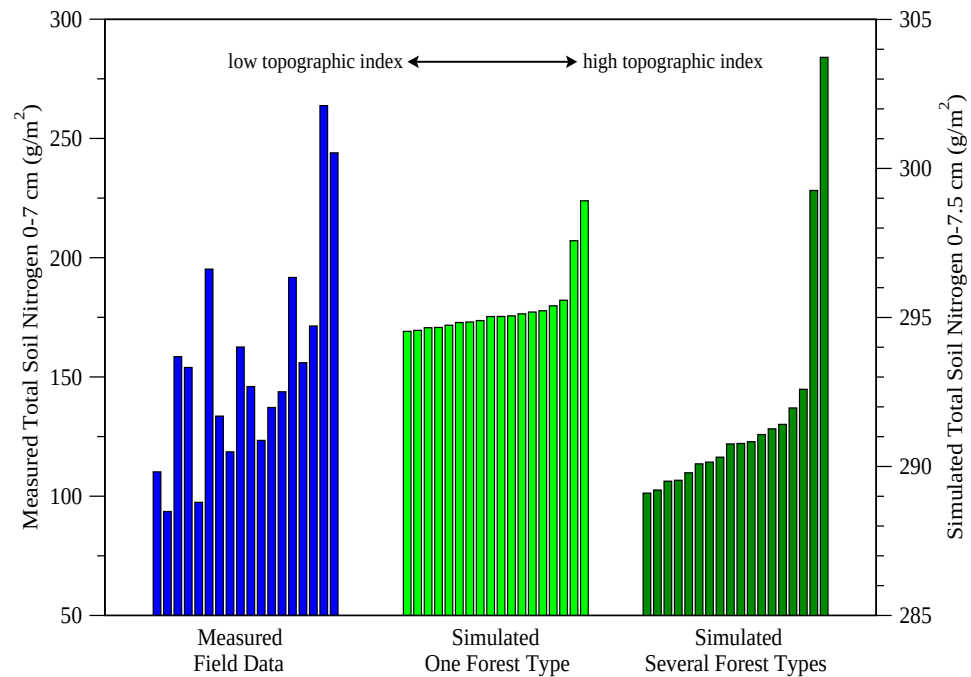


Figure 17: Comparison of total soil nitrogen for Walker Branch Watershed.

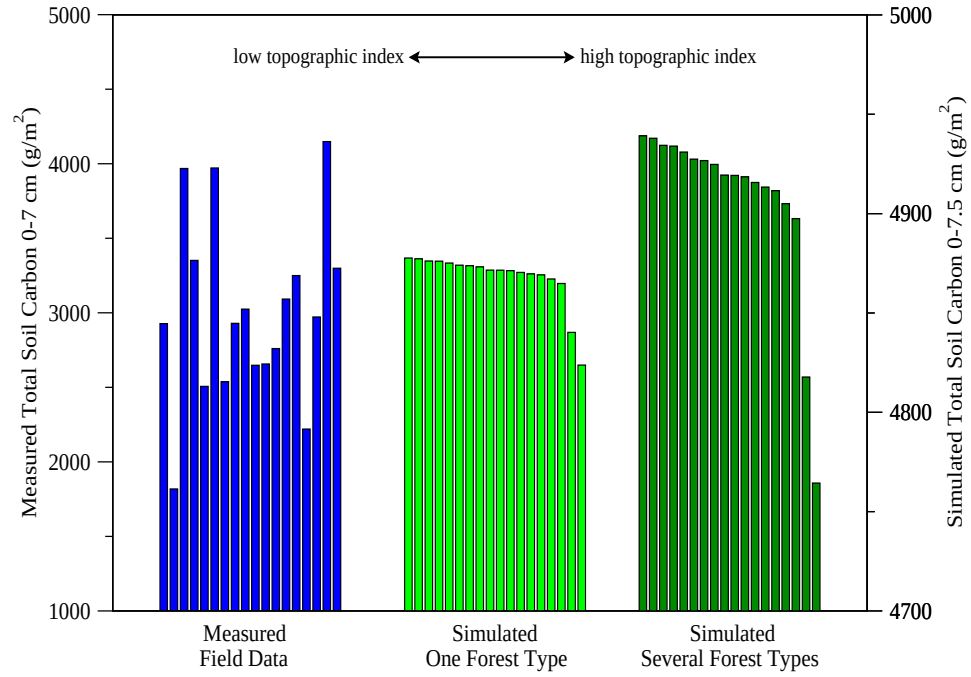


Figure 18: Comparison of total soil carbon for Walker Branch Watershed.

was, on average, two times greater than the field data, and the total soil carbon model output was approximately 1.6 times of that in the field data.

In general, the difference in the numerical values between the field and simulated data could be due to the long time evolution of the soil and to the diverse pattern of disturbance that has occurred on the Walker Branch Watershed (see Figure 3), especially when it is compared with a 13-year simulation that assumed the starting conditions were the same over the entire watershed. A long term simulation, over 100 years, would allow the nitrogen and carbon pools in the model to stabilize and improve the soil patterns both numerically and with respect to the topographic trends. Furthermore, finding the soil parameters that best reflected the landuse history of Walker Branch Watershed was difficult. Either the parameters were not available, or they were collected at only one point in time and space, making difficult the conditioning of TOPDNDC.

Figure 19 presents the comparison between the measured and simulated values for the soil ammonium in each of the seasons at the West Fork Catchment. Figure 20 shows the same comparison, but for soil nitrate.

The simulated soil ammonium and nitrate showed a seasonal pattern across topographic indices very similar to that observed in the measured data. The seasonal pattern of ammonium and nitrate results from the changing balance between nitrogen uptake by plants and nitrogen mineralization by microbes. Nitrogen does not accumulate in inorganic (mineral) forms. Ammonium is either taken up by the plants and soil microbes or nitrified to nitrate. Nitrate is either taken up or leached from the soil. When plants are growing, they uptake large amounts of mineral nitrogen from the soil; when they are not growing (fall and winter seasons) the mineral nitrogen tends to increase in the soil. Microbial activity is directly related to soil temperature and moisture.

Soil ammonium is strongly correlated with topographic index [*Garten et al., 1994*], but that is not the case for soil nitrate in all seasons. Hence, the simulated patterns for soil ammonium tended to follow more closely those of the measured data than the ones for soil nitrate.

Of the two different simulations performed with TOPDNDC, the one with the same type of forest covering the entire watershed showed the smallest differences in the soil parameters across topographic indices. However, it is important to note that even when starting from a totally uniform landscape, except for soil moisture distribution, the model was capable of producing realistic patterns of nutrients and growth in only 13 years of simulation.

The TOPDNDC simulation with different types of forest distributed over the watershed according to topographic index showed a larger difference in the soil parameters values between topographic indices. Having a forest with different physiological characteristics, in this case leaf C:N ratio and potential relative growth rate,

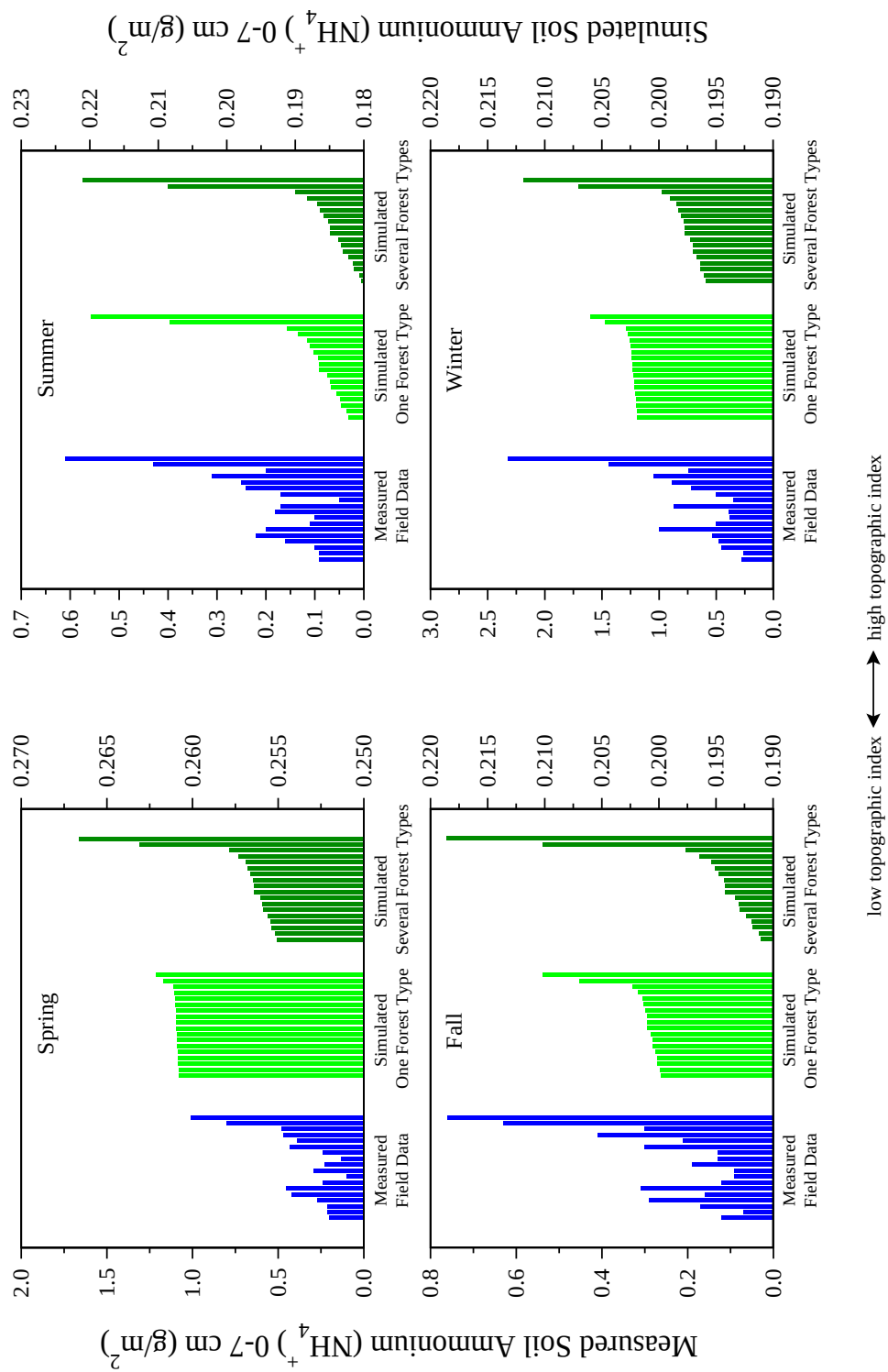


Figure 19: Comparison of soil ammonium for Walker Branch Watershed.

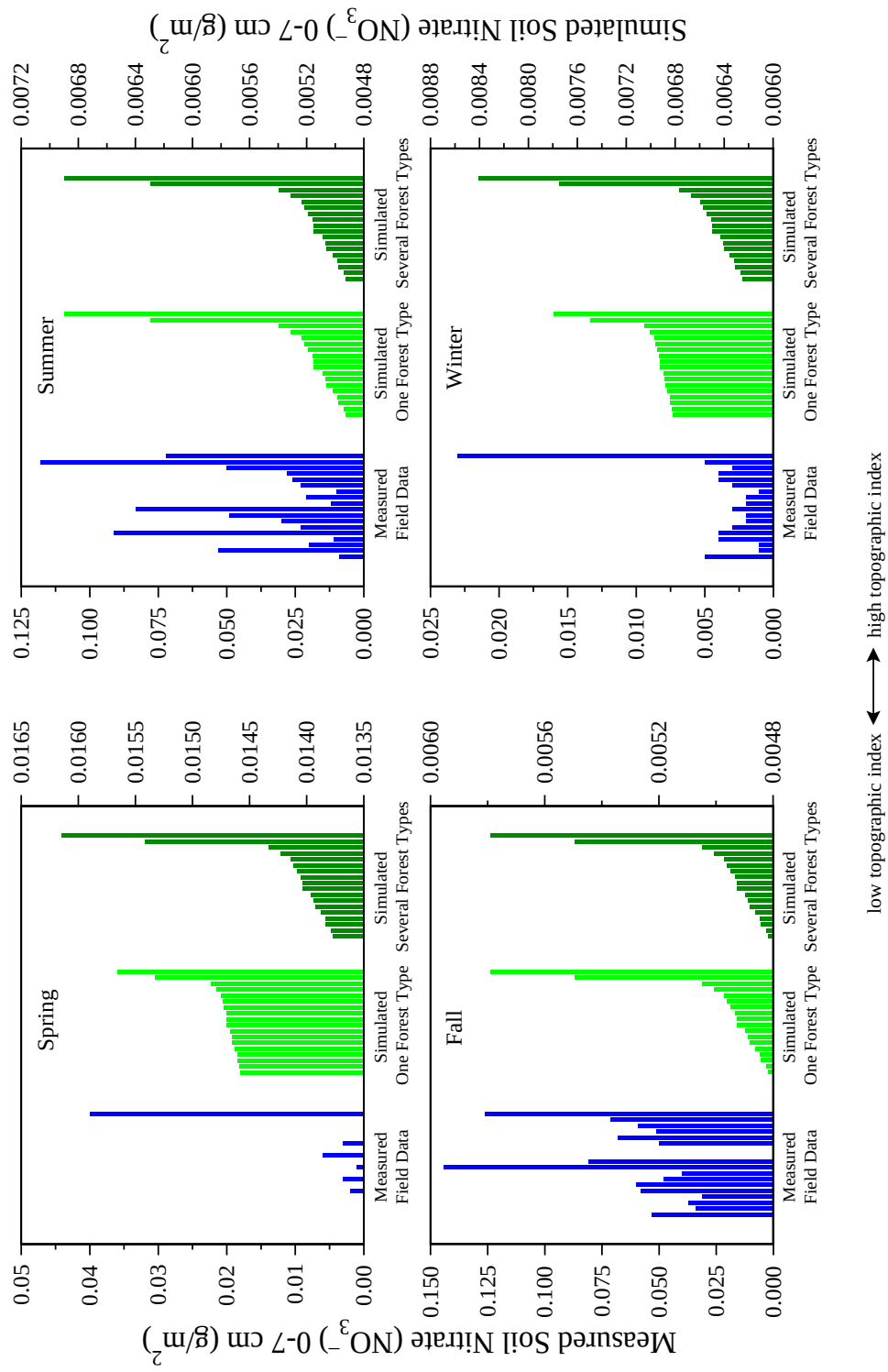


Figure 20: Comparison of soil nitrate for Walker Branch Watershed.

has a greater effect on soil composition than just the soil moisture. The greater effect is due to the cycling of nutrients, in this case, nitrogen. The leaves of the forest on the ridges (low topographic index), the dry part of the watershed, have a higher leaf C:N ratio than the leaves on the valleys (high topographic index) and slopes (intermediate topographic index). During leaf-fall, less nitrogen is deposited on the forest floor of ridges and, therefore, less is available for growth during the next growing season. It is important to note that although TOPDNDC distributes water laterally within the watershed, this water does not carry any leached nutrients with it. Nutrients that are leached are lost to the soil-plant-watershed system.

A correlation analysis between the measured and simulated data for the West Fork Catchment is presented in Table 18. The correlations were performed to have a quantitative evaluation of the patterns resulting from the simulations. The correlation coefficients for the two different simulations were identical, which could be an artifact of the very small variation ranges of the simulated output in comparison to the measured data.

Table 18: Correlation between measured and simulated values for Walker Branch Watershed.

Soil Parameter	Correlation Coefficient (r)	
	with Respect to Measured Values	
	One Forest Type	Several Forest Types
Total Carbon	-0.34	-0.34
Total Nitrogen	0.80	0.80
Ammonium (NH_4^+)		
spring	0.90	0.90
summer	0.92	0.92
fall	0.90	0.90
winter	0.92	0.92
Nitrate (NO_3^-)		
spring	0.78	0.78
summer	0.54	0.54
fall	0.49	0.49
winter	0.83	0.83

The total soil nitrogen had a high correlation coefficient, whereas the total soil carbon had a low and inverse correlation with the field data. The correlation for ammonium performed by season showed strong correlations ($r \geq 0.90$) for all seasons. The nitrate correlations, also performed by seasons, showed smaller correlations especially for the summer and fall seasons, but all correlations were positive. All these correlations were in agreement with the results presented previously in a graphical manner.

Figure 21 presents the live trunk biomass production for the two simulations at the West Fork Catchment of the Walker Branch Watershed.

The lower tree growth on the drier sites (low topographic index) can be explained by the lower availability of water that supplies nitrogen for growth. In the case of the different forest types in the watershed, this effect is compounded by the reduced return of nitrogen from the fallen leaves C:N ratio, and by the relative

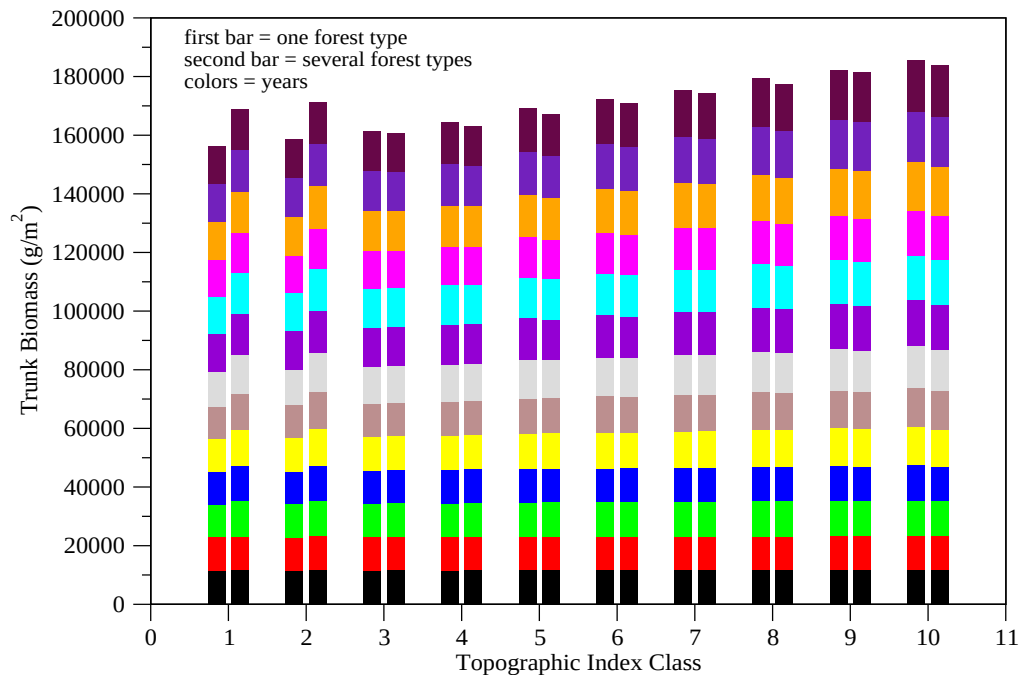


Figure 21: Simulated live trunk biomass across topographic index classes for Walker Branch Watershed.

growth rate associated to this C:N ratio. The higher productivity (growth) of the pine trees on the ridges (topographic index classes 1 and 2) can be explained by their leaf C:N ratio. Pine trees had larger leaf C:N ratios than the other trees, therefore in the model, they produced larger amounts of carbon (biomass) with the same amount of soil nitrogen, and were less limited in their growth by nitrogen.

Figure 22 shows the simulated live trunk biomass increment for both simulations. As can be seen in this figure, the difference between biomass production in the driest (low topographic index) and wettest (high topographic index) sites increased with time, and was very similar for both types of simulations. Both simulations showed the same variability in the biomass across the topographic index, except for the fast growing pines on the ridges. There were no field data available for comparison to the tree trunk growth simulations.

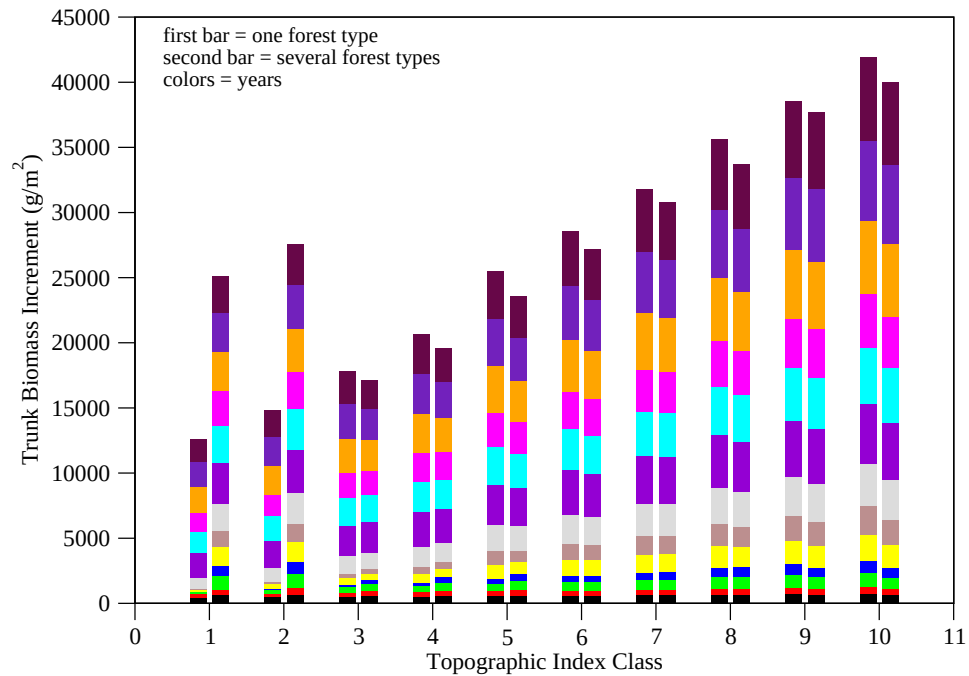


Figure 22: Simulated live trunk biomass increment across topographic index classes for Walker Branch Watershed.

Chapter 5

Conclusion and Further Development

5.1 Conclusion

Understanding how vegetation-resource interactions vary across watersheds is critical for accurately predicting the rate of ecosystem processes, since vegetation growth is limited more often by unfavorable environmental conditions than by limitations in the capacity of the physiological processes [*Kozlowski et al., 1991*]. Accordingly, TOPDNDC attempts to model the spatial and temporal dynamics of carbon and nitrogen in small catchments in grasslands and temperate forests.

The first part of the study consisted of the improvement and testing of the lumped biogeochemical component of the ecohydrological model. The biogeochemical component was parameterized for a flat grassland, where all of the water flow was assumed to be vertical. The repeated process of simulation, comparison, and modification of the model allowed the improvement of the biogeochemical part of the model.

The improved version of the biogeochemical model had a high correlation coefficient of 0.85 with respect to the measured data, whereas the original version of the model had a lower correlation of 0.79. A linear regression of the simulated versus measured data for the improved version had a slope of 0.84 and an r^2 of 0.71. The slope of the original version of the model versus the measured data was significantly

lower at 0.37 and had a correspondingly low r^2 of 0.62. Furthermore, the improved version of the model was able to not only model the mean behavior of the data, as the original version of the model did, but was also capable of reproducing a large proportion of the temporal variability in the field data, where the original version could not.

The grassland field data consisted of the summed dry mass of 207 plots with different plant species growing on them, while the model simulates one species at a time. This may obscure some of the growth patterns in comparison with the model. Modeling multiple species could yield better predicted results for the grassland. However, total biomass is more relevant than individual species because species abundance is affected by competition as well as climate. Nonetheless, the model showed that the patterns of biomass production may ultimately be explained by the variation of nutrients and water affecting plant growth instead of the level of biodiversity present in the plot, which is the explanation of the authors that collected and analyzed the grassland data [*Tilman et al.*, 2001].

The second part of the study established a link between the improved biogeochemical component and a semi-distributed hydrological component that apportioned the biogeochemical processes in the watershed according to soil moisture and added the lateral distribution of water. Field data collected along a transect in a watershed that included ridges and valleys were compared with the model simulation.

The results of this model simulation revealed that the model was able to reproduce the same patterns found in the field data, and that in seven out of ten cases had high correlations ($r \geq 0.78$) with respect to the field data. The intention of the simulation was not to obtain a perfect match with the measured values, but to predict more detailed patterns of carbon and nitrogen in the catchment. The simulation period was short and assumed that the starting soil carbon and nitrogen were the same everywhere in the catchment. However, soils are complex systems

continually evolving according to the changes in the environment, and a longer time simulation of 100 or 200 years may yield results even closer to the field data.

Grassland and forest ecosystems behave differently. Precipitation fluctuations have strong effects on grassland productivity, but relatively small effects on forest growth [*Knapp and Smith, 2001*]. New or modified processes may be needed to improve forest simulations because the processes currently implemented in the model may not be completely applicable to forests. It is the lateral distribution of water in a watershed that makes the forest simulation more complex. The hydrological link between the lateral and vertical distribution components of the model was kept relatively simple, which may be another source of the discrepancy between the model results and the field data. A more complex vertical redistribution of the water would result in better forest simulations.

There have been few published studies of models that simulate biomass production at the small catchment scale, and even fewer models that simulate biomass production and soil nutrient dynamics in small catchments. TOPDNDC is a step in the direction of a more precise spatial and temporal ecohydrological model.

5.2 Further Development

The development of models is not a static process. As confidence is gained in existing models, new questions are asked and new models developed to answer these questions. No single model is adequate for all questions. But modeling is an important tool for testing hypotheses that can lead to a better understanding of the natural world.

The model presented in this study attempts to explain the processes that control the movements of basic nutrients and water in grasslands and forests. The model can be further developed and improved from the lessons here learned.

The model can be improved in two different manners, by increasing the speed of execution and modularity of the models in general, and by modifying particular existing routines to better represent the physical processes described by them.

The biogeochemical component of the model was not written in a modular fashion, making it difficult to add or exchange modules describing key ecological or hydrological processes. Converting the biogeochemical component to a modular structure will facilitate model comparisons and greatly increase the versatility of the model.

Improvement in the computational speed of the model can be achieved by converting it to a complete vectorized form within PV-Wave, the current platform development. PV-Wave is an array-oriented programming language and, therefore, is optimized for array processing. The hydrological component of the model is already in vectorized form, but the biogeochemical component is not in that form. Vectorization of the model is not easily accomplished, and some processes may not be convertible. However, the reduction in processing time can be substantial. Currently, TOPDNDC processing time is about one hour for ten years of simulation in a mid-to-high-end PC (Intel PIII CPU, 750 MHz), but this processing time can be reduced by a factor of five if the entire model is set up in vectorized form.

The hydrological component of TOPDNDC is not set up for long term simulations. The entire hourly precipitation record is read into memory at the beginning of the simulation, which limits the period of simulation to the amount of memory available in the computer. Reading the hourly precipitation record every year of the simulation instead of only once per simulation would allow long term simulations to proceed without computer hardware limitations.

Several possible improvements to the hydrological component of the model were identified. Adding the capability to run multiple instances of TOPMODEL

would allow TOPDNDC to divide the watershed into subwatersheds, giving TOPDNDC more flexibility in characterizing the behavior of the whole watershed.

Incorporating aspect, the direction that a surface faces, into the hydrological component of TOPDNDC would allow the model to perform more realistic simulations. Aspect has a strong influence on evapotranspiration rates, and it has been shown to influence the distribution of nutrients in humid, temperate watersheds [*Garten et al., 1994*].

Adding a snowpack-snowmelt routine to the hydrological component of TOPDNDC would increase the applicability of the model to areas where snow plays an important hydrological role.

Both of the evapotranspiration equations utilized by TOPDNDC (Thornthwaite and Hamon) are temperature based formulations. Although these equations require a reduced set of parameters to determine evapotranspiration, they tend to underestimate evapotranspiration and are not applicable to arid and semi-arid areas [*Xu and Singh, 1998*]. Better evapotranspiration formulations exist like the Penman-Monteith equation. However, they require a large number of field parameters, which are only available for certain areas in the US. Its addition to TOPDNDC would allow a better determination of evapotranspiration rates when such field data are available.

The hydrological component of TOPDNDC does not model infiltration. It assumes that all water infiltrates the soil. This assumption is acceptable for the field sites that were modeled in this study, which have high infiltration rates. However, the addition of an infiltration routine to the model will make it more applicable to other areas.

The biogeochemical component of TOPDNDC could also be improved with the addition or modification of several routines. One of the most important routines to add would be a photosynthesis module. The model does not simulate photosynthesis explicitly. Adding this module would make the model more physically based

and produce better simulations, since photosynthesis, productivity, and evapotranspiration are tightly linked in nature.

The root respiration module in the current model is simplistic and not linked to plant growth. A better root respiration module may have a more realistic impact on plant growth and provide better estimates of CO₂ production.

The biogeochemical component of the model does not consider the translocation of nutrients from the leaves to the roots before senescence. However, it does consider the opposite mechanism, the translocation of nutrients from the roots to start leaf growth. The translocation from leaves to roots is an important plant process for conserving resources instead of losing them to the soil during leaf fall [*Larcher*, 1995]. The addition of this process would involve the creation of carbon pools for roots and trunk, and would improve the nutrient cycling in the model.

A very important modification to the model would consist of the improvement of the linkage between the hydrological and biogeochemical components of TOPDNDC. The current linkage is a simple approach to the transfer of water between the two components. A more sophisticated linkage would not assume that the water is distributed equally among all soil layers, and would include a better connection between the saturated and unsaturated zones on the hydrological component of the model.

Performing a sensitivity analysis of the different parameters in TOPDNDC would assist in understanding the complex behavior of TOPDNDC and determining the key parameters in the model. These key parameters should be obtained with the least amount of uncertainty possible for their use in the model.

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Appendix

Nomenclature

Biogeochemical Model (DNDC)

$Q_{i,i-1}$	flow of water per unit area from layer i-1 down to layer i
$K_{i,i-1}$	average hydraulic conductivity of layers i and i-1
h_i	hydraulic head for level i
z_i	depth of layer i
ϕ_i	water tension for layer i
ϕ_{sat}	saturated water tension
θ_i	layer i water content
β	soil water parameter
W_*	water content where retention curve has inflection (0.92)
m_1	soil water parameter
m_2	soil water parameter
$store_{intcp}$	canopy water interception storage
$store_{intcp_{max}}$	maximum canopy water interception storage
LAI	leaf area index
PET	potential evapotranspiration
T_a	mean monthly air temperature
I	annual heat index
PT	potential transpiration
$Plant_{water\ req.}$	daily plant water requirement
$Plant_{daily\ carbon}$	daily plant carbon uptake
$q_{i,i-1}$	heat flux from layer i-1 down to layer i
$k_{i,i-1}$	average thermal conductivity of layers i and i-1
T_i	temperature for level i
k_{min}	mineral soil thermal conductivity

n	soil porosity
k_{water}	water thermal conductivity
k_{org}	organic matter thermal conductivity
$PMBY$	potential maximum biomass yield
$PMGY$	potential maximum growth yield
G_f	fraction of crop biomass C in grain C pool at harvest
$PMNU$	potential maximum nitrogen uptake
$C : N$	carbon to nitrogen ratio
t_{fg}	fraction of the growing season elapsed
N_{up}^*	potential daily nitrogen uptake
N_{crop}	nitrogen crop content
C	carbon pool
t	time
μ_{clay}	clay content reduction factor
μ_{CN}	C:N ratio reduction factor
μ_{Tm}	combined temperature and moisture reduction factor
S	labile fraction of organic C compounds in the pool
k_l	specific decomposition rate of labile fraction
k_r	specific decomposition rate of resistant fraction
AM	accumulated NH_3 loss at time t
D	diffusion coefficient
$dNNO$	NH_4^+ converted to NO_3^-
K_{35}	nitrification rate at 35 °C
$\mu_{T,n}$	temperature reduction factor for nitrification
$\mu_{m,n}$	moisture reduction factor for nitrification
B	total biomass of denitrifier
u_{DN}	relative growth rate of the denitrifiers

$u_{N_xO_y}$	relative growth rate of NO_3^- , NO_2^- , or N_2O denitrifiers
$\mu_{pHN_xO_y}$	soil pH reduction factor on NO_3^- , NO_2^- , or N_2O transformation rate
μ_T	soil temperature reduction factor
pH	potential of hydrogen
$K_{c,1/2}$	half-saturation value of soluble carbon
$K_{N_xO_y,1/2}$	half-saturation value of NO_3^- , NO_2^- , or N_2O
N_xO_y	concentration of NO_3^- , NO_2^- , or N_2O in soil water
M_c	maintenance coefficient of carbon
Y_c	maximum growth yield on soluble carbon
C_{con}	consumed soluble carbon
CO_2	CO_2 production
$C_{con,t}$	total consumption of soluble carbon
$\left(\frac{dB}{dt}\right)_g$	potential growth rate of denitrifier biomass
$M_{N_xO_y}$	maintenance coefficient of NO_3^- , NO_2^- , or N_2O
$Y_{N_xO_y}$	maximum growth yield on NO_3^- , NO_2^- , or N_2O
N	total nitrogen as NO_3^- , NO_2^- , or N_2O
CNR	carbon to nitrogen ratio of denitrifiers
$\left(\frac{dN}{dt}\right)_{asm}$	nitrogen assimilation rate by denitrifiers
P_{N_2}	emitted fraction of the total N_2 evolved in a day
P_{N_2O}	emitted fraction of the total N_2O evolved in a day
AD	adsorption factor depending on clay content in the soil
PA	air-filled fraction of the total porosity
DI	daily growth rate
CN_l	carbon to nitrogen ratio of leaves
$EnvC$	environmental conditions (soil moisture, soil temperature, and air temperature)
CDD	cumulative degree-days

d_g	number of growth days
T_{air}	daily mean air temperature
$T_{plant_{thld}}$	minimum threshold air temperature
NH_4^+ _{ads}	ammonium adsorption by soil
CEC	cation exchange capacity
SOM	soil organic matter
N_{month}	number of days in a month
H_{day}	hours of sunlight during a day
ϕ_{lat}	latitude of location
sun_d	sun declination
$days_{year}$	number of days in a year
$days_{elapsed}$	number of days elapsed

Hydrological Model (TOPMODEL)

q_{total}	total flow per unit area
$q_{overland}$	saturation overland flow per unit area
$q_{subsurface}$	subsurface flow per unit area
q_{direct}	flow due to direct precipitation on saturated areas, per unit area
q_{return}	return flow from subsurface areas, per unit area
A	surface area of hillslope slice
R	spatially uniform recharge rate
T	transmissivity
T_{max}	transmissivity when the soil is saturated
c	contour width or length
β	angle of hillslope with respect to the horizontal
K_z	saturated hydraulic conductivity

K_0	hydraulic conductivity at the soil surface
f	rate of decrease of K with depth
z_{wt}	depth of water table
z_D	depth to bedrock
s	saturation deficit
ϕ	fraction of soil porosity
m	scaling parameter
a	contributing area for water flow
$\bar{s}$	average saturation deficit
i	number of hillslopes in a catchment
λ	mean topographic index
A_{sat}	water saturated area
P	precipitation
L	length of all stream channels
Z_{rz}	effective root zone depth
S_{rmax}	maximum available root zone storage
θ_{fc}	soil moisture content at field capacity
θ_{wp}	soil moisture content at wilting point

Vita

Born and raised in Mexico City, Enrique Gomezdelcampo earned his Bachelor of Science in Engineering Physics from the Universidad Iberoamericana. He worked for several years in computer consulting until he decided to change careers. He completed his Master of Science in Environmental Engineering in 1991 at the University of Tennessee, with the help of a research assistantship at the Tennessee Valley Authority Engineering Laboratory. He then moved to Seattle, Washington where he completed two quarters of graduate work, which led to a job in Delft, The Netherlands in groundwater research. Having worked in surface water and groundwater issues and problems, he decided to try wastewater too, and moved back to Mexico City to work for a British water company. A few years later, needing more challenges and fresh air, he moved back to the University of Tennessee to pursue a Ph.D. related to hydrology. Having reached the end of his academic career as a student, he is now thinking of trying the other side as a professor.