A model of nitrous oxide evolution from soil driven by rainfall events: 1. Model structure and sensitivity

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A Model of Nitrous Oxide Evolution From Soil Driven by Rainfall Events:

1. Model Structure and Sensitivity

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This paper describes a rain-event driven, process-oriented simulation model, DNDC, for the evolution of nitrous oxide (N$_2$O) emissions from agricultural soils. The model consists of three submodels: thermal-hydraulic, decomposition, and denitrification. Basic climate data drive the model to produce dynamic soil temperature and moisture profiles and shifts of aerobic-anaerobic conditions. Additional input data include soil texture and biochemical properties as well as agricultural practices. Between rainfall events the decomposition of organic matter and other reaction oxidations (including nitrification) dominate, and the levels of total organic carbon, soluble carbon, and nitrate change continuously. During rainfall events, denitrification dominates and produces N$_2$O and N$_2$. Daily emissions of N$_2$O and N$_2$ are computed during each rainfall event and cumulative emissions of the gases are determined by including nitrification N$_2$O emissions as well. Sensitivity analyses reveal that rainfall patterns strongly influence N$_2$O emissions from soils but that soluble carbon and nitrate can be limiting factors for N$_2$O evolution during denitrification. During a year sensitivity simulation, variations in temperature, precipitation, organic C, clay content, and pH had significant effects on denitrification rates and N$_2$O emissions. The responses of DNDC to changes of external parameters are consistent with field and experimental results reported in the literature.

1. INTRODUCTION

This paper reports the structure of a computer model for assessing nitrous oxide (N$_2$O) emissions from agricultural soils. The current atmospheric N$_2$O concentration is about 8% greater than in the preindustrial era and is increasing at a rate of about 0.8 ppb (0.25%) per year [Weiss, 1981; Elkins and Rossen, 1989]. Ice core measurements indicate that the concentration of atmospheric N$_2$O started to increase around the period 1700-1800 [Pearman et al., 1986; Khalil and Rasmussen, 1988; Etheridge et al., 1988], with a rapid concentration increase beginning about 1950 [Intergovernmental Panel on Climate Change (IPCC), 1990].

Nitrous oxide is a nonreactive, long-lived, radiatively active trace gas in the troposphere. Currently, N$_2$O contributes approximately 5% of the global warming potential in greenhouse effect assessments [Rodhe, 1990]. The major sink for N$_2$O is photolysis in the stratosphere, leading to nitrogen oxide products which influence levels of stratospheric ozone [Crutzen, 1970]. Because of these important links to both climate and atmospheric chemistry the causes for the increasing atmospheric N$_2$O concentration are of great interest. International discussions are already in progress to develop approaches for regulating the sources of N$_2$O. Unfortunately, the large uncertainties present in estimates of sources of N$_2$O preclude the development of any detailed strategies for their mitigation.

A recent assessment of N$_2$O sources by the IPCC indicates that soils and agriculture fertilizers are important sources of N$_2$O [IPCC, 1990]. Nitrous oxide is primarily derived as an intermediate product of microbial denitrification and nitrification processes in soils (for reviews see Delwiche [1981]; Sahrawat and Keeney [1986]; Seiler and Conrad [1987]). While many laboratory and field investigations of N$_2$O production rates by soil microbes have been conducted, quantification of global N$_2$O emissions from soils has proven extremely difficult because of the heterogeneity of soil chemical, physical, and biological properties which interact to determine production and emission rates. In particular, variations in soil moisture, soil texture, and carbon and nitrogen substrates for microbial nitrification and denitrification are critical to determining N$_2$O emissions [e.g., Leffelaar and Wessel, 1988; Tanji, 1982; Frissel and Van Veen, 1981; Batlach and Tiedje, 1981; Cho et al., 1979]. Numerous simulation models have been developed to estimate denitrification rates and processes in soils (Table 1). The early models [e.g., Focht, 1974; Mehran and Tanji, 1974] were studies of denitrification kinetics at the laboratory-incubation scale. Several of the more recent models [e.g., Grant, 1991; Johnson et al., 1991; Clay et al., 1985; and Molina et al., 1983] were designed to predict total N losses from soils on field scales, but not specifically N$_2$O fluxes to the atmosphere, and thus model only total denitrification (N$_2$O + N$_2$) in combination with various decomposition processes. Others, which focus more closely on N$_2$O by modeling the various steps of denitrification and microscopic processes such as substrate diffusion [e.g., Leffelaar and Wessel, 1988; McConnaughey and Bouldin, 1985], do not incorporate field scale variables such as temperature, moisture, and carbon substrate availability. Van Veen and Frissel [1979] model both decomposition and denitrification processes, substrate diffusion and availability.
and various inorganic N transformations but do not treat denitrification with enough detail to separate N\textsubscript{2}O from N\textsubscript{2} production. The model of Parton et al., [1988; also see Mosier and Parton, 1985] focuses on the relative importance of denitrification and nitrification to N\textsubscript{2}O fluxes in grasslands and takes into account daily to seasonal variations in soil conditions but does not contain enough detail concerning substrate dynamics to be easily generalizable to a variety of agricultural ecosystems. None of these models are able to predict daily or seasonal N\textsubscript{2}O emissions from field soils using readily available input data. In particular, none of these models can be used to study the impacts of various agricultural practices on nitrous oxide emissions.

To better understand and quantify soil sources of N\textsubscript{2}O, we have developed a model that couples decomposition and denitrification processes, as influenced by the soil environment, to predict emissions from agricultural soils (Figure 1). The model runs on a personal computer and uses commonly available climate, soil, and agricultural practice data as input. Our model is directed to two applications: (1) investigation of the interactions of fundamental climatic, pedologic, agronomic, and microbiological variables which influence the production and emission of nitrous oxide from agricultural soils and (2) development of an improved quantitative assessment of the large-scale emissions of nitrous oxide from agroecosystems in the United States and globally.

2. MODEL

2.1. Model Framework

Emissions of nitrous oxide and dinitrogen (N\textsubscript{2}) from soils are not temporally continuous. On the basis of field monitoring and experimentation, pulses of N\textsubscript{2}O and N\textsubscript{2} from soils are observed to follow rainfall or irrigation events [Roulier and Fetter, 1973; Duxbury and McConnaughey, 1986; Mosier et al., 1986; Saxstone et al., 1985; Goodroad...
and Keeney, 1984]. The connection between emissions of N$_2$O and N$_2$ and rain events can be explained primarily through the biochemical processes related to microbial activities in soils.

Denitrification occurs under oxygen-deficient conditions (e.g., in wet soils following rain events), when denitrifying bacteria utilize nitrate (rather than oxygen) as an electron acceptor [e.g., Knowles, 1981; Sahrawat and Keeney, 1986; Davidson, 1991]. Dissolved carbon compounds (referred to below as soluble carbon) in the soil solution are the major electron donors during denitrification as carbon is converted to CO$_2$. Under oxic conditions, these denitrifying bacteria along with many other bacteria decompose organic residues and microbial biomass to produce soluble carbon compounds and ammonium. These two processes along with ammonia volatilization, nitrification, adsorption, and plant uptake interact to control the substrate pools for microbial activity and gaseous emissions of N$_2$O, N$_2$, and CO$_2$.

Because of the substantial difference in N$_2$O emissions between wet and dry soils, a season or year can be modeled effectively as a sequence of wet and dry periods. Soil temperature and moisture are two key factors controlling the rates of both decomposition and denitrification during these periods. Soil thermal-hydraulic flux, aerobic decomposition, and denitrification submodels of DNDC (DeNitrification and DeComposition) work together in simulating N$_2$O and N$_2$ emissions with a 1-day time step (1 hour during rain events) (Figure 1). In addition, the model calculates concentrations of nitrate, nitrite, ammonium, organic residues, microbial biomass, humads, and soluble carbon in the soil profile, as well as mineralization rates of C and N, nitrate leaching, and emissions of carbon dioxide and ammonia from the soil.

Model equations and parameters are presented in the appendices.

### 2.2. Submodel of Thermal-Hydraulic Flows

A one-dimensional soil heat flux and moisture flow model (Figure 2) has been designed to calculate average hourly and daily soil temperature and moisture profiles. The modeled soil is divided into a series of horizontal layers. Each layer is assumed to have a uniform temperature and moisture content, assigned to a point at the middle of the layer. For each time step, water fluxes and heat flows between layers are determined by the gradients of soil water potential and soil temperature, respectively. All values are determined per unit area in the horizontal plane. These gradient-driven equations are numerically modeled by explicit finite difference equations (see Table 2 for thermal-hydraulic model equations). Typical vertical spatial resolution is 5 cm and time steps are generally about 30 min. Rainwater is added or evaporated and water removed at the beginning of each time step, before gradient-driven fluxes are determined. Water flow out of the bottom of the modeled profile (typically 50 cm deep) is driven by gravity drainage only [Van Bavel and Lascano, 1980]. Heat flux into/out of the bottom layer is determined by the gradient between the bottom layer temperature and the annual mean air temperature imposed at 500 cm depth. To run the simulation with a minimum amount of meteorological input data, the heat flux at the soil surface is simplified to a gradient driven flux between the soil surface, which is assigned a temperature equal to the mean daily air temperature, and the top soil layer temperature at a depth of several centimeters.
Fig. 2. The one-dimensional thermal-hydraulic submodel simulates soil heat flux and moisture flow and calculates hourly and daily average soil temperature and moisture profiles. The heat fluxes and moisture flows are driven by diffusion gradients (and gravity for water flow) for a layered soil profile. Soil texture controls soil hydraulic properties.

The moisture boundary condition at the soil surface has precipitation/irrigation and evapotranspiration components. Precipitation (or irrigation) events are prescribed input events. Since the goal of the DNDC model is to predict seasonal or annual \( \text{N}_2\text{O} \) emissions, the precise timing of precipitation events is not important. We assume that all rain events start at midnight, are of constant intensity (throughout an individual storm but potentially varying intensity from one storm to the next), and of variable duration. At the beginning of each time step, the rainfall for that time step saturates the soil, layer by layer, to the depth that it can fill. Any residual rainwater (not needed to fill a layer) is uniformly distributed in the next deeper layer. At present we assume there is no surface runoff, and although evaporation of intercepted water can account for a significant fraction of rainwater, particularly for vegetation with a thick canopy [Bras, 1990], we do not model intercepted water.

Evapotranspiration (ET) is calculated as monthly average values using the Thornthwaite formula, in which potential ET is determined by monthly mean air temperature and then adjusted for daylight length relative to 12 hours [Dunne and Leopold, 1978]. If soil moisture is limiting then actual ET is less than potential ET. We follow Sellers [1965] in having actual ET decrease linearly from potential ET to zero as the soil water potential drops from -0.033 MPa (field capacity) to -1.5 MPa (wilting point). DNDC assumes that ET

**TABLE 2. Thermal-Hydraulic Submodel Equations**

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q_{li} = -K_{li} \frac{(T_i - T_{zi})}{(z_i - z_{zi})} )</td>
<td>Soil heat flux (layer ( i-1 ) to ( i ))</td>
</tr>
<tr>
<td>( Q_{li} = \frac{K_{li} \phi_{li}}{T_i} )</td>
<td>Soil heat flux at bottom of profile</td>
</tr>
<tr>
<td>( \phi = \phi_{li}(\theta_i)^{n}, \text{if } \theta &lt; W_e )</td>
<td>Water retention relation</td>
</tr>
<tr>
<td>( \phi = -m_i(W - m_i)(W - 1), \text{if } \theta \geq W_e )</td>
<td></td>
</tr>
<tr>
<td>( dT_i = dT_1(T_i - T_{min})/(\alpha e) )</td>
<td>Soil heat flux at surface</td>
</tr>
<tr>
<td>( k_i = (1 - n)k_{low} + n \theta_i k_{mom} )</td>
<td>Soil relative hydraulic conductivity</td>
</tr>
<tr>
<td>( k_i = (1 - n)k_{low} + n \theta_i k_{mom} )</td>
<td>Soil thermal conductivity</td>
</tr>
<tr>
<td>( E/\alpha = \theta_i/(\alpha e) )</td>
<td>Energy conservation</td>
</tr>
<tr>
<td>( E = E_{li} )</td>
<td>Soil layer volumetric heat capacity</td>
</tr>
</tbody>
</table>

**TABLE 3. Soil Type and Properties**

<table>
<thead>
<tr>
<th>Soil Type</th>
<th>Clay</th>
<th>( K_{sat} )</th>
<th>( \phi_{sat} )</th>
<th>( \theta_{b} )</th>
<th>( \theta_{wp} )</th>
<th>c</th>
</tr>
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<tbody>
<tr>
<td>Sand</td>
<td>3</td>
<td>39.5</td>
<td>1.056</td>
<td>4.05</td>
<td>3.50</td>
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<tr>
<td>Loamy sand</td>
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<td>0.938</td>
<td>4.38</td>
<td>1.78</td>
<td>30</td>
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<td>Sandy loam</td>
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<td>0.208</td>
<td>4.90</td>
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<td>45</td>
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<tr>
<td>Silty loam</td>
<td>14</td>
<td>48.5</td>
<td>0.043</td>
<td>5.30</td>
<td>56.6</td>
<td>46</td>
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<tr>
<td>Loam</td>
<td>19</td>
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<td>0.042</td>
<td>5.39</td>
<td>14.6</td>
<td>55</td>
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<td>Sand cl loam</td>
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<td>0.038</td>
<td>7.12</td>
<td>8.63</td>
<td>59</td>
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<tr>
<td>Silt cl loam</td>
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<td>47.7</td>
<td>0.010</td>
<td>7.75</td>
<td>14.6</td>
<td>66</td>
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<tr>
<td>Clay loam</td>
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<td>47.6</td>
<td>0.015</td>
<td>8.32</td>
<td>36.1</td>
<td>76</td>
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<tr>
<td>Sandy clay</td>
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<td>42.6</td>
<td>0.013</td>
<td>10.4</td>
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<td>Silty clay</td>
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<td>17.4</td>
<td>75</td>
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<tr>
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<td>77</td>
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<tr>
<td>Organic</td>
<td>80</td>
<td>80.0</td>
<td>0.010</td>
<td>7.75</td>
<td>14.6</td>
<td>66</td>
</tr>
</tbody>
</table>

See notation section for definitions of variables. Source: Specific heats (c), de Vries [1975]. \( \theta_b \) and \( \theta_{wp} \) calculated (see text). All other values, Clapp and Hornberger [1978]. Note: \( K_{sat} \) and \( \beta \) values for organic soil are not reported by Clapp and Hornberger [1978]; we chose the values for silty clay loam.
removes water from the top 20 cm of the soil; root density is assumed uniform over the top 20 cm, and root growth dynamics are modeled. For each layer, actual ET withdrawal depends on that layer's water content.

DNDC characterizes soil physical properties by soil texture (see Table 3 for soil parameters), following the work of Clapp and Hornberger [1978]. The soil thermal conductivity depends on soil water content and on the type of soil (mineral or organic). The soil layer net thermal conductivity for a given moisture content is an average of the thermal conductivities of the solid phase and water, weighted by their relative volumes in the soil.

Soil water tension and unsaturated hydraulic conductivity are strong functions of the soil water content. For each of these, DNDC uses the exponential formulation of Clapp and Hornberger [1978], with representative parameters for each of 12 soil textures.

2.3. Submodel of Decomposition

When soil is in an aerobic state, decomposition and other oxidation reactions, including nitrification, are the dominant microbial processes. Assimilation of inorganic carbon and nitrogen into microbial biomass also occurs with the decomposition of residues, microbial biomass and humads (materials partially stabilized by humification and adsorption, McGill et al., [1981]). During decomposition and assimilation, organic C, soluble C, ammonium, and nitrate are produced and may accumulate. The levels of these substrates depend on the balance between the rates of mineralization (transformation of organic C or N to inorganic C or N), assimilation, and loss (plant uptake, sorption, or volatilization).

The decomposition submodel follows that of Molina et al., [1983], with three active carbon pools for the decomposition sequence (Figure 3). The soil profile is divided into horizontal layers with a typical thickness of 2 cm. Each layer is assumed to have uniform properties (temperature, moisture, substrate and microbe concentrations, etc.) and all decomposition calculations are performed layer by layer. The decomposition submodel runs in a daily time step for every day of the simulation. When a rain event occurs, the decomposition submodel pauses, and the denitrification submodel runs until the top 20 cm of the soil has an average water content of less than 40% of porosity [Bremner and Shaw, 1958a, b; Nommik, 1956], or for a maximum of 10 days by which time very little denitrification occurs in the model due to depletion of substrates. The decomposition submodel then resumes with the rainy day and the average soil climate for that rainy day.

Pools of organic matter. Decomposition (as modeled in DNDC) can simultaneously occur in three organic matter pools: decomposable residues (mainly plant residues), microbial biomass, and humads; each pool has a labile and resistant component (Figure 3). The passive organic phase, or stable humus, is assumed not to interact with the active phase during the short time span of the model (about 1 year). We define soil organic carbon as the sum of microbial biomass, humads, and humus. During the decomposition process each component decomposes independently [Hunt, 1977; Jenkinson, 1977].

Decomposition rates. The resistant and labile carbon pools

![Soil temperature & moisture from submodel of thermal-hydraulic flow](image)

**Fig. 3.** In the decomposition submodel, organic matter consists of four pools: residue, microbial biomass, humads, and passive humus. Nonhumus pools contain labile and resistant components. Components have different temperature- and moisture-dependent decomposition rates. Pools of soluble carbon, microbial biomass, and nitrate are shared with the denitrification submodel.
The clay content of soils also affects the decomposition of organic matter; clays can adsorb organic C and shelter it from decomposition [Bouwman, 1990]. DNDC models this shielding effect as a multiplicative factor (0.35 to 1.67; 1.0 for loam) that decreases the decomposition rate for increasing clay contents.

**Production and decomposition of microbial biomass and humads.** As the residue pools decompose, the carbon released is either respired as CO₂ or incorporated into microbial biomass (Figure 3). DNDC first determines the amount of CO₂ produced. From this and a microbial efficiency value, DNDC calculates the amount of carbon incorporated into microbial biomass, with 90% going into labile biomass and 10% going into resistant biomass [Gilmour et al., 1985]. Microbial efficiency, defined here as the ratio of C assimilated into microbial biomass to residue C released by decomposition, has been reported to vary between 20% and 60% [Paul and Juma, 1981; Paul and Van Veen, 1978; Chichester et al., 1975; Molina et al., 1983; Gilmour et al., 1985]. In soils amended with easily decomposable organic material (e.g., animal wastes), the microbial population buildup is high [Griffin and Laine, 1983], while in unamended soils the fraction of decomposed C used for microbial growth is relatively small [Jansson and Persson, 1982]. This study adopts efficiency values of 60% for amended soil and 20% for unamended soil.

As microbes die and their biomass decomposes (Figure 3), 20% of the carbon is transferred to CO₂, 60% of the carbon is reincorporated into new microbial biomass, and 20% is transferred to the resistant humads pool [Molina et al., 1983; Gilmour et al., 1985]. The resistant humads pool can lose carbon through decomposition or via soil disturbance (see discussion of tillage effects below). As each humads pool decomposes, 40% of the carbon is transferred to the stable humus pool, 40% of the carbon is converted to CO₂ and 20% is reincorporated into microbial biomass [Molina et al., 1983].

The soluble carbon pool (Figure 3) consists of the carbon from microbial biomass decomposition (60%) and humads decomposition (20%) that is recycled into microbial biomass. Thus it is not actually a carbon pool but rather an indicator of the daily rate of decomposition. When a rain event occurs, the denitrification model initiates its calculations using this soluble carbon pool as the amount of soluble carbon available in the soil.

**Effect of temperature and moisture on decomposition.** DNDC models the effects of soil temperature [Nyhan, 1976] and water content [Clay et al., 1985] on microbial activity with reduction factors which retard the decomposition rate for nonoptimum conditions (Figures 4a and 4b). These relationships between microbial activity and both temperature and moisture are generally consistent with the results of other studies [e.g., Bremner and Shaw, 1958a, b; Witkamp, 1966; Alexander, 1971; Myers and McGrady, 1971; Jager and Bruins, 1974; Wildung et al., 1975]. Since the reduction factor represents the combined effect of temperature and moisture, it is taken as the product of the two factors.

**Nitrogen behavior during decomposition.** During the decomposition of organic matter in soils, nitrogen behavior is simulated in the following manner: (1) when organic C is oxidized to CO₂, the associated N is transformed to ammonium (NH₄⁺); (2) NH₄⁺ can be nitrified to nitrate or transferred to ammonia and volatilized to the air; and (3)
Volatilization of ammonia is related to the N\(_2\)O concentration; ammonia to ammonia is influenced by soil pH, content in soils [Jones, 1972; Food and Agriculture Organization (FAO)/UNESCO, 1971-1981], clay content is chosen as an index of adsorption sites. Transformation of NH\(_4\)+ by clay and organic matter in soil are the rough positive correlation between clay and organic carbon content in soils [Jones, 1972; Food and Agriculture Organization (FAO)/UNESCO, 1971-1981], clay content is chosen as an index of adsorption sites. Transformation of ammonium to ammonia is influenced by soil pH and transfers to ammonium. Nitrification. Under aerobic conditions, NH\(_4\)+ can be oxidized to NO\(_3\)- and NO\(_2\)- by ammonium oxidizers [McGill et al., 1981; Van Veen and Frissel, 1979]. This process is called nitrification. According to a study by Watts and Hanks [1978] the potential rate of nitrification in the surface soil is related to the available NH\(_4\)+, soil temperature, and soil moisture. DNDC models the rate as a function of these factors with an optimal rate at 35°C and soil pore moisture content of 90% [Hadas et al., 1986; Figures 4a and 4b].

During nitrification the amount of N\(_2\)O emitted in soils correlates with the amount of nitreizable N in soils [Parton et al., 1988; Bremner and Blackmer, 1978]. In DNDC we regard ammonium as the direct factor controlling N\(_2\)O emissions under aerobic conditions. On the basis of the data of Bremner and Blackmer [1981], N\(_2\)O emissions from nitrification processes are modeled as a function of soil temperature and soil ammonium concentration.

2.4. Submodel of Denitrification

Leffelaar and Wessel [1988] present a detailed model of denitrification processes in laboratory incubations of soil samples. Denitrification follows the reduction sequence (NO\(_3\)- → NO\(_2\)- → N\(_2\)O → N\(_2\)) with the rate of each process depending on the availability of the particular N oxide and all processes competing for available C. DNDC uses a similar model structure for denitrification (Figure 5), activating this submodel at every rainfall event. The soil profile is divided into horizontal layers with a typical thickness of 2 cm. Each layer is assumed to have uniform properties (temperature, moisture, substrate and microbe concentrations, etc.) and all denitrification calculations are performed layer by layer. In DNDC a rainfall event is defined as the time period from rainfall initiation to the time when relative moisture (fraction of pores occupied) decreases to 40%. In the model, denitrifying conditions (low oxygen availability) occur immediately upon saturation with water. During the denitrification calculation we assume that only denitrifiers are active.

Relative growth and death rates of denitrifiers. Almost all
denitrifiers are capable of anaerobic growth only in the presence of $\text{NO}_3^-$, $\text{NO}_2^-$, or $\text{N}_2\text{O}$. The growth rates of denitrifiers directly affect the reduction rates of these nitrogenous oxides. Denitrifiers are assumed to become active at the onset of a rainfall event. Tiedje [1978] and Smith and Tiedje [1979] reported a short lag period (1 to 10 hours) before denitrification began following soil wetting. Ignoring this lag time probably causes DNDC to model $\text{N}_2\text{O}$ and $\text{N}_2$ production earlier than in field situations.

The growth rates of the bacteria are taken to be proportional to their respective biomass (Van Veen and Friesel [1981]; see Table 6 and Table 7 for denitrification submodel equations and parameters, respectively). Relative growth rates, which depend on the concentrations of carbon and electron acceptors (N oxides), are calculated with double-Monod kinetics, a simple function describing multiple-nutrient-dependent Michaelis-Menten-type growth [Bader, 1978]. Following Leffelaar and Wessel [1988] we assume that the relative growth rates for denitrifiers with different substrates are independent; competition among the bacteria takes place via the common soluble carbon substrate.

The denitrifier death rate is modeled as proportional to denitrifier biomass. The C and N from dead cells are added to the pools of immobilized C and N and no longer participate in the dynamic processes [Leffelaar and Wessel, 1988]. Since denitrifier biomass is a very small fraction of total soil biomass, this represents an insignificant loss of C and N from the soil system.

Effect of soil environment on denitrification. The effect of soil pH on denitrification has been measured by many researchers [Mueller et al., 1980; Klemedtsson et al., 1978; Burford and Bremner, 1975; Stanford et al., 1975; Khan and Moore, 1968; Wijler and Delwiche, 1954]. On the basis of experimental studies, pH affects nitrate and nitrous oxide transformation rates differently such that at low pH (<5), most denitrification stops at $\text{N}_2\text{O}$ [Focht, 1974; Leffelaar and Wessel, 1988]. In general, total denitrification decreases as soil pH decreases.

An exponential relationship between denitrification rate and temperature has been observed (e.g., Focht, 1974; Nommik, 1956; Dawson and Murphy, 1972). According to Bailey and Beauchamp [1973] and Nommik [1956] the rate of denitrification is very temperature dependent in the $10^\circ-35^\circ\text{C}$ range, with a $Q_{10}$ near 2.0 [Stanford et al., 1975; Knowles, 1981]. The rate continues to increase at higher temperatures, reaching a maximum at $60^\circ-75^\circ\text{C}$ and then falling to zero.
when a soil layer is initially saturated with water, diffusion of gases in soils and to the air-filled porosity of the soil. Based on the chemical composition of the denitrifier biomass, NO\textsubscript{3}\textsuperscript{-} denitrifier + NO\textsubscript{2}\textsuperscript{-} denitrifier + N\textsubscript{2}O denitrifier [Volfelaar and Wessel, 1988].

On the basis of the growth rates of denitrifiers and the C:N ratio in the bacteria the assimilation of N during to deeper layers with the water flux. In the model, N:O and carbon consumed and the amount used for cell synthesis.

Nitrate, nitrite, and nitrous oxide consumption are calculated with Pirt's equation. Carbon dioxide production is calculated as the difference between the total amount of carbon consumed and the amount used for cell synthesis.

Since denitrification mostly occurs within the top 30-75 cm for most mineral soils [Gilliam et al., 1978; Roiston et al., 1976; Khan and Moore, 1968], a typical total thickness of a modeled soil profile is 50 cm. Initially, the top 10 cm of soil is assumed to be chemically uniform. Below this level, the concentrations of organic residues, organic C and NO\textsubscript{3} decrease exponentially with depth (50% every 10 cm). During rainfall events, dissolved NO\textsubscript{3} and NO\textsubscript{2} move down to deeper layers with the water flux. In the model, N\textsubscript{2}O and N\textsubscript{2} do not move with the water flux. The thermal-hydraulic

<table>
<thead>
<tr>
<th>TABLE 7. Denitrification Parameters</th>
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<tbody>
<tr>
<td>Parameter</td>
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</tr>
<tr>
<td>$M(NO)$</td>
</tr>
<tr>
<td>$Y_c$</td>
</tr>
<tr>
<td>$Y_{\text{max,NOD}}$</td>
</tr>
<tr>
<td>$Y_{\text{max,NOD}}$</td>
</tr>
<tr>
<td>$R$</td>
</tr>
<tr>
<td>$R^{BO}$</td>
</tr>
<tr>
<td>$FD$</td>
</tr>
</tbody>
</table>

3. MODEL OPERATION

TABLE 8. Model Input Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Climate</td>
<td>Mean daily air temperature; rainfall events (timing, intensity, duration); NO\textsubscript{3} concentration in rainfall.</td>
<td></td>
</tr>
<tr>
<td>Soil</td>
<td>Type (texture); density; pH; initial residue, organic carbon, nitrate, and ammonium contents; initial soil temperature and moisture.</td>
<td></td>
</tr>
<tr>
<td>Land use</td>
<td>Crop type; seeding and harvest time.</td>
<td></td>
</tr>
<tr>
<td>Agronomic practices</td>
<td>Tillage (timing, intensity); fertilizer application (species, amount, timing, depth); manure amendment (type, amount, timing); irrigation (amount, timing); crop rotation (crop types, rotation pattern).</td>
<td></td>
</tr>
</tbody>
</table>
submodel starts the simulation by assuming a soil with uniform temperature and water content profiles.

The model output includes daily moisture and temperature profiles, concentrations of residues, organic carbon, microbial biomass, soluble carbon, NH$_4^+$, NO$_3^-$, NO$_2^-$, N$_2$O, and N$_2$ in the profile, and emissions of N$_2$O, N$_2$, NH$_3$, and CO$_2$ from the soil.

4. Sensitivity Analysis

To test the response of the sub-models and the complete model to variations of relevant parameters from baseline conditions, four sensitivity analyses were conducted: (1) the sensitivity of soil moisture to soil texture and rainfall patterns; (2) the sensitivity of decomposition to drying period duration, soil temperature, soil moisture, initial residue, and organic C; (3) the sensitivity of denitrification to soil-soluble C, nitrate, and rainfall duration; and (4) the sensitivity of total model behavior for an annual simulation to variations in soil properties, initial organic C, annual precipitation, and temperature.

In order to unravel the complex behavior of DNDC our sensitivity analyses were conducted by varying one parameter and fixing others during one cycle. This sensitivity analysis does not validate the model but demonstrates that the model behavior is consistent with its structure and assumptions, as described in section 2. Model validations against field measurements are reported in a companion paper [Li et al., this issue].

4.1. Soil Moisture and Rainfall Patterns:
The Thermal-Hydraulic Submodel

The DNDC model illustrates the importance of soil moisture to both denitrification and decomposition. This section examines two tests of the sensitivity of the thermal-hydraulic submodel to soil texture and imposed precipitation/irrigation conditions, one to rainfall intervals and the other to rainfall amounts.

In the first test the thermal-hydraulic submodel was run for five different rainfall patterns spread over a 90-day period: (1) 1.25 cm of rain in 5 hours every 4 days, (2) 2.50 cm of rain in 5 hours every 8 days, (3) 3.75 cm of rain in 5 hours every 12 days, (4) 5.00 cm of rain in 5 hours every 16 days, and (5) 6.25 cm of rain in 5 hours every 20 days. The total rainfall was the same for each simulation. For each soil type the amount of time the soil was dry (water content < 40% water-filled pore space) and the amount of time the soil was wet (water content > 65% water-filled pore space) increased as the rainfall interval increased, while the time that the soil was at an intermediate water content decreased (Figure 6). Other things being equal, we would expect N$_2$O emissions to increase as both rainfall interval and duration increased.

Two simulation studies examined the effects of increased rain amounts for evenly spaced storms (10-day intervals): one varied rainfall intensity and the other varied rainfall duration. Both had the expected effect of increasing the amount of time the soils were quite wet (>65% pore space occupied) and decreasing the amount of time the soils were dry. For all thermal-hydraulic submodel tests, sandier soils were drier than the clayey or organic soils in any particular simulation.

4.2. Soluble Carbon and Nitrate Availability in Soil:
The Decomposition Submodel

Both soluble C and NO$_3^-$ are the products of decomposition and other oxidation reactions in soils. In DNDC the levels of the two substrates reflect the interactions of several factors, including initial organic residues, total organic carbon, soil moisture and temperature, and decomposition duration. In this section we examine the sensitivity of the decomposition submodel, which generates soluble carbon and

<table>
<thead>
<tr>
<th>Item</th>
<th>Decomposition Submodel</th>
<th>Denitrification Submodel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil type</td>
<td>loam</td>
<td>loam</td>
</tr>
<tr>
<td>Soil density</td>
<td>1.5 g/cm³</td>
<td>1.5 g/cm³</td>
</tr>
<tr>
<td>Soil pH</td>
<td>7.0</td>
<td>7.0</td>
</tr>
<tr>
<td>Soil temperature</td>
<td>20°C</td>
<td>20°C</td>
</tr>
<tr>
<td>Initial residue*</td>
<td>10 g C/kg soil</td>
<td>10 g C/kg soil</td>
</tr>
<tr>
<td>Initial organic C*</td>
<td>10 g C/kg soil</td>
<td>10 g C/kg soil</td>
</tr>
<tr>
<td>Initial soluble C*</td>
<td>100 mg N/kg soil</td>
<td>100 mg N/kg soil</td>
</tr>
<tr>
<td>Initial ammonium</td>
<td>5 mg N/kg soil</td>
<td>5 mg N/kg soil</td>
</tr>
<tr>
<td>Nitrate in rainwater</td>
<td>0.5 cm/h</td>
<td>1 mg N/l</td>
</tr>
<tr>
<td>Rainfall duration</td>
<td>10 hours</td>
<td>5 hours</td>
</tr>
<tr>
<td>Rainfall intensity</td>
<td>0.5 cm/h</td>
<td>1 mg N/l</td>
</tr>
</tbody>
</table>

*Decomposable residues, including plant residues and microbial polysaccharides,

Active organic carbon, including microbial biomass and humids,

Water-soluble carbon.

Effect of initial residue and organic carbon content. As the initial organic residue content increased from 0 to 0.1 kg C/kg soil, the production of soluble carbon also increased (Figure 8). Nitrate levels increased up to 0.05 kg C/kg soil but then decreased slightly with further increases of organic carbon. This slight decrease in the C-rich soil is related to the high population of microbial organisms (which follows from the higher initial organic carbon values); the microbes assimilate nitrate as it is produced by decomposition.

Effect of decomposition period duration. Under the standard conditions, the soil nitrate content increased linearly as the decomposition period was extended, due to continuing nitrification of the ammonium released by decomposing organic matter. The soluble carbon level did not change since carbon decomposition and assimilation into microbial biomass reached a steady state (Figure 9).

Effect of soil climate. Soluble carbon and NO₃⁻ reached maximum values when the water-occupied fraction was fixed at about 60% of the total porosity; both wetter and drier conditions limited the production of soluble carbon and NO₃⁻ (Figure 10). As the soil temperature increased from 0°C to 30°C, soluble carbon and nitrate increased. Above 40°C, soluble carbon gradually decreased and nitrate sharply decreased and then increased (Figure 11). At temperatures above 45°C (not normally found in field soils) the production of CO₂ decreased because of the depression of microbial activity. Nitrification ceases above 45°C, so no nitrate is produced, but the reduction in nitrogen assimilation due to
suppressed microbial activity means that more of the initial nitrate pool remains after the 30-day decomposition period.

**Effect of initial ammonium concentration on N\textsubscript{2}O emissions.**

N\textsubscript{2}O emissions from nitrification are modeled as a function of soil water ammonium concentration, soil temperature, and soil moisture. The response of the model to changes in the initial ammonium concentrations is large but temporary (Figure 12). Within 1 week all cases converged on a stable low level of 0.5 g N ha\textsuperscript{-1} d\textsuperscript{-1}. This value is a function of soil temperature, moisture, and the rate of NH\textsubscript{4}\textsuperscript{+} production through decomposition processes.

### 4.3. Emissions of N\textsubscript{2}O During A Rainfall Event: The Denitrification Submodel

During normal model operation the denitrification submodel receives substrate status information from the decomposition submodel at the beginning of each rain event. For this sensitivity study, the denitrification model was run alone using standard conditions (Table 9).

**Effect of soluble carbon and nitrate contents.** Soluble C and NO\textsubscript{3}\textsuperscript{-} are the main substrates necessary to keep denitrifiers active under anaerobic conditions. As the initial value of soluble carbon increased, the rise in total denitrification (N\textsubscript{2}O+N\textsubscript{2}) depended on the initial content of NO\textsubscript{3}\textsuperscript{-} in soils (Figure 13). For NO\textsubscript{3}\textsuperscript{-} levels below about 30 mg N/kg soil and soluble carbon greater than 10 mg C/kg soil, nitrate limited total denitrification. Increasing soluble C can decrease N\textsubscript{2}O emission because it lowers the ratio of N\textsubscript{2}O/NO\textsubscript{3} produced by supplying sufficient carbon substrate to complete the denitrification process (Figures 14 and 15). If the content of soluble carbon is fixed, increasing the initial NO\textsubscript{3}\textsuperscript{-} content will not necessarily increase N\textsubscript{2}O emissions (Figure 15). Thus the relationship between N\textsubscript{2}O emission and the soluble carbon and NO\textsubscript{3}\textsuperscript{-} contents in the soil appears to be quite complex. These results are consistent with numerous observations which indicate (1) water-soluble carbon is highly correlated with denitrification activity and (2) increasing carbon availability generally decreases the ratio of N\textsubscript{2}O/NO\textsubscript{3} [Burford and Bremner, 1975; Smith and Tiedje, 1979; Focht and Verstraete, 1977; Nornmik, 1956; and Delwiche, 1959]. These relationships between soluble carbon and nitrate could be important for reducing N\textsubscript{2}O emission during normal model operation the denitrification submodel to be quite complex. These results are consistent with numerous observations which indicate (1) water-soluble carbon is highly correlated with denitrification activity and (2) increasing carbon availability generally decreases the ratio of N\textsubscript{2}O/NO\textsubscript{3} [Burford and Bremner, 1975; Smith and Tiedje, 1979; Focht and Verstraete, 1977; Nornmik, 1956; and Delwiche, 1959]. These relationships between soluble carbon and nitrate could be important for reducing N\textsubscript{2}O emission.
4.4. Annual $N_2O$ Emissions: The DNDC Model

The complete DNDC model was tested for its sensitivity to various climate and soil parameters over a 1-year simulation. A set of standard climate/soil conditions was developed, based on the climate and soils of Iowa [United States Department of Agriculture (USDA) 1989, 1967]. In order to determine the effects of different climate or soil properties on annual emissions of $N_2O$, annual simulations were conducted by varying each parameter by $\pm 20\%$ while holding the others fixed (Table 10). The results of this analysis show that the sensitivities of total denitrification ($N_2O+N_2$), $N_2O$ emissions, and CO$_2$ emissions to the climate/soil parameters are quite different (Figure 17). None of these sensitivity studies test the model sensitivity to different agricultural practices.

Annual total denitrification. Variations in annual precipitation had the greatest effect on the annual total denitrification (see Figure 17a); when annual precipitation was increased by 20%, total denitrification increased by more than 50%. Higher precipitation keeps the surface soil under anaerobic conditions for a longer time, enhancing denitrification. Soil pH had the second largest effect. When soil pH was reduced from 6.0 to 4.8, the annual denitrification rate decreased by 40%; denitrifiers are very sensitive to a low pH environment. When the mean annual temperature or initial total organic C were increased by 20%, total denitrification also increased by about 20%. Higher temperatures stimulate denitrifier and decomposition activity; higher organic C provides more substrates (soluble C and nitrate) to support the growth of denitrifiers. Changes in soil density, clay content, rainfall nitrate, initial soil nitrate, and initial soil ammonium had slight to no effect on total denitrification. Rainfall nitrate at these levels (0.8-1.2 mg N/L) is a small nitrate source (6 kg N/ha/yr) relative to modeled nitrification at this site (286 kg N/ha/yr).

Annual $N_2O$ emission. Because the ratio of $N_2O$ production to total denitrification ($N_2O+N_2$) depends on many factors, the behavior of the annual $N_2O$ emissions is different from that of total denitrification (Figure 17b). Soil texture (clay content) and density had the greatest effect on $N_2O$ emissions. When soil clay content was decreased by 20%, the annual
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![Graph showing effect of rainfall duration on N₂O and N₂ flux. Modeled N₂O and N₂ emissions increase linearly with an increase in rainfall duration when carbon and nitrate substrates do not limit denitrification.](image)

Fig. 16. Effect of rainfall duration on N₂O and N₂ flux. Modeled N₂O and N₂ emissions increase linearly with an increase in rainfall duration when carbon and nitrate substrates do not limit denitrification.

N₂O emissions increased by more than 40%. This phenomenon is due to the stronger adsorption by clays of N₂O than of N₂; the model clay content was changed without changing the soil hydraulic properties, so soil moisture changes had no effect here. Since we defined soil organic C as kg C per kg soil, an increase in soil density automatically causes an increase in organic C. An increase in organic C will increase the microbial biomass which tends to increase N₂O production more than N₂ production because of the time constraints set by various wet periods. Thus the N₂O/(N₂O+N₂) ratio generally rises.

In the same vein an increase in annual precipitation greatly increased annual N₂ emission but slightly reduced N₂O emission (Figure 17); anaerobic conditions last longer, allowing denitrification processes to continue more toward completion (N₂ rather than N₂O). When soil temperature was increased by 20%, the annual N₂O emissions increased by 14% because of enhanced microbial activity. Annual N₂O emissions decreased slightly with either an increase or a decrease in soil pH reflecting the optimal pH range for N₂O production. Nitrate concentration in rainfall, initial soil nitrate, and initial ammonium had little to no effect on annual N₂O emissions.

**Annual CO₂ emission.** Total organic C strongly influenced annual CO₂ emissions (Figure 17c) because the soil microbial pool size varies directly with total organic carbon. The same effect occurs with a change in soil density (g soil/cm³). Soil clay content showed a large inverse effect on annual CO₂ emission; clays can adsorb organic C and shield it from decomposition. When soil temperature was increased (decreased) by 20%, annual CO₂ emissions increased (decreased) by 13%, reflecting the general dependence of microbial activity on temperature. An increase in annual precipitation had a negative impact on annual CO₂ emissions. Rates of decomposition are slowed with the increased frequency/duration of anaerobic conditions. Soil pH, nitrate

| TABLE 10. Standard Conditions and Variations for Sensitivity Analysis on DNDC Model |
|---------------------------------|------------------|------------------|
| Item                           | Standard         | Variation        | Unit               |
| Annual rainfall events         | 24               | 29 - 21          | cm                 |
| Annual precipitation           | 82.5             | 99.1 - 66.0      | cm                 |
| Annual average temperature     | 9.1              | 10.9 - 7.3       | °C                 |
| Nitrate content in rain        | 1.0              | 1.2 - 0.8        | mg N/l             |
| Soil clay content              | 34%              | 40% - 27%        |                   |
| Soil density                   | 1.4              | 1.68 - 1.12      | g/cm³              |
| Soil pH                        | 6.0              | 7.2 - 4.8        |                   |
| Initial total organic C        | 0.03             | 0.036-0.024      | g C/kg             |
| Initial soil nitrate           | 10               | 12 - 8           | mg N/kg            |
| Initial soil ammonium          | 10               | 12 - 8           | mg N/kg            |

*Heavy and intermediate rainfalls,
\[\text{Including plant residues, microbial polysaccharide, and other organic matter.}\]

Fig. 17. Sensitivity of N₂O+N₂, N₂O and CO₂ emissions to increasing or decreasing input parameters by 20% in a loam soil in Iowa, USA. Changes in environmental parameter values (+20% from standard conditions; see Table 4) cause variations in (a) annual total denitrification (N₂O+N₂) flux, (b) annual N₂O flux, and (c) annual CO₂ flux.
content in rainfall, initial soil nitrate, and initial ammonium all had little or no effect on annual CO₂ emissions.

5. SUMMARY AND CONCLUSIONS

This paper describes a process-oriented rain-event model of soil nitrogen and carbon biogeochemistry that has been developed to predict N₂O emissions from agricultural soils over a growing season. A soil thermal-hydraulic model propagates a surface climate (daily mean air temperature and precipitation/irrigation) into the soil to determine soil temperature and moisture profiles. A decomposition submodel tracks the soluble carbon and nitrogen pools in the soil as plant residues decompose and soil microbes grow and die. A rain-event-initiated denitrification submodel calculates N₂O and N₂ production while the soil is wet during and following rain/irrigation events. The model allows for cropping, fertilizer and organic matter additions, and soil tillage so that agricultural practices can be simulated.

We performed a series of sensitivity studies of the total model and the three submodels to determine the factors which have strong effects on the behavior of DNDC and its three submodels (Table 11). Although the specific sensitivities depended on somewhat arbitrary standard conditions and variations, we feel that the model behavior (for N₂O evolution, total denitrification, and CO₂ emissions) is representative of what is (or would be) observed in the field. What these sensitivity studies do not portray are the impacts of agricultural land use practices and the interactions of the various processes as several factors change at once, as would happen when comparing different agroecosystems. Only through studying the complex interactions among soil climate, decomposition and denitrification processes, and agronomic practices can a complete picture of agroecosystem scale nitrous oxide fluxes begin to emerge. A companion paper reports the comparison of DNDC simulations to field studies [Li et al., this issue].

Since most fundamental biogeochemical processes have been included in DNDC, it can potentially serve not only for estimating N₂O emissions but also for other processes related to mass exchange between soil systems and the atmosphere, such as fertilizer efficiency, carbon balance in soils, CH₄ and CO₂ emissions, nitrogen leaching, and groundwater pollution.

NOTATION

**Thermal-Hydraulic Submodel Variables**

- \( a \): ET parameter \( (= 0.49 \pm 0.07)^{-1} \cdot 7.71 \cdot 5^{-1} \cdot 6.75 \cdot 7^{-1} \)
- \( c_s \): specific heat of material \( x \), \( 1 \text{ kg}^{-1} \text{ °C}^{-1} \)
- \( D_{AY} \): 1/12 of the day's hours of daylight.
- \( d_0 \): change in the water content of soil layer \( i \), cm.
- \( f \): drainage factor \( (f \text{ is presently fixed at } 1.0) \)
- \( h_i \): hydraulic head for level \( i \), cm.
- \( I \): ET parameter \( (= C_{m, \text{min}}^{-1} \left(T_i^*/55\right)^{-1}) \), °C.
- \( k_{min} \): minimal soil thermal conductivity \( (0.0259) \), \( J \text{ cm}^{-1} \text{ °C}^{-1} \)
- \( k_i \): average thermal conductivity of layers \( i \) and \( i-1 \), \( J \text{ cm}^{-1} \text{ °C}^{-1} \)
- \( k_{organic} \): organic matter thermal conductivity \( (0.0025) \), \( J \text{ cm}^{-1} \text{ °C}^{-1} \)
- \( k_{water} \): water thermal conductivity \( (0.0057) \), \( J \text{ cm}^{-1} \text{ °C}^{-1} \)
- \( K_{l, i} \): average hydraulic conductivity of layers \( i \) and \( i-1 \), cm s⁻¹.
- \( K_{sat} \): saturated hydraulic conductivity, cm s⁻¹.
- \( l_i \): thickness of layer \( i \), cm.
- \( m_1 \): parameter \( (= y_{1} \cdot (1-W_{2})^{-2} - y_{2} \cdot \beta/W_{2} \cdot (1-W_{2})^{-1}) \), cm.
- \( m_2 \): parameter \( (= 2 \cdot W_{1} - y_{1} \cdot \beta/(m_{1} \cdot W_{1})) \)
- \( n \): soil porosity.
- \( N_i \): number of days in the month.
- \( \rho_{soil} \): heat flux from layer \( i-1 \) down to layer \( i \), J cm⁻².
- \( \rho_{water} \): flow of water per unit area from layer \( i-1 \) down to layer \( i \), cm s⁻¹.
- \( t_i \): time, s.
- \( T_i \): temperature for level \( i \), °C.
- \( T_{mean} \): mean annual air temperature, °C.
- \( T_{mean} \): mean monthly air temperature of month \( n \), °C.
- \( W_i \): water content where retention curve has inflection (0.92).
- \( z_a \): depth where temperature variation assumed negligible (500), cm.
- \( z_o \): depth of layer \( i \) (positive down from surface), cm.
- \( \beta \): soil water parameter (range = 4 to 11.4).
- \( a \): material density, kg m⁻³.
- \( \Theta_{l, i} \): layer \( i \) water content (fraction pore volume occupied).
- \( \Theta_{sat} \): soil water content at field capacity.
- \( \Theta_{sata} \): soil water content at the plant wilting point.
- \( \Theta_{water} \): water tension parameter, cm.
- \( \phi_{water} \): soil water tension at the inflection point, cm.

**Decomposition Submodel Variables**

- \( AM \): accumulated NH₃ loss at time \( t \), mol cm⁻².
- \( B \): total microbial biomass produced, kg C.
- \( CLAY \): soil clay fractional content.
- \( CLAY_{max} \): maximum clay fraction in model soils (0.63).
- \( COP \): CO₂ respired during residue decomposition, kg C.
- \( D \): C production by potential residue decomposition, kg C ha⁻¹ d⁻¹.
- \( D_{diff} \): diffusion coefficient \( (0.025) \), cm² d⁻¹.
- \( d_{NO} \): NH₄⁺ converted to NO₃⁻, kg N ha⁻¹ d⁻¹.
- \( eff \): microbial efficiency for decomposing residues.
- \( FIXNH₄ \): proportion of adsorbed NH₄⁺.
- \( k_i \): specific decomposition rate (SDR) of labile fraction, d⁻¹.
- \( k_s \): SDR of the resistant fraction, d⁻¹.
- \( K_{diss} \): dissociation constant for NH₄⁺-NH₃ equilibrium.
- \( K_{HNO} \): dissociation constant for H⁺-OH⁻ equilibrium.
Denitrification Submodel Variables

\[ K_{\text{ad}} \text{ nitrification rate at 35°C (25), mg kg}^{-1} \text{ soil d}^{-1} \]
\[ NH_3 \text{ NH}_3 \text{ concentration in liquid phase, mol cm}^{-3} \]
\[ NH_4^- \text{ NH}_4^- \text{ concentration in liquid phase, mol L}^{-1} \]
\[ NH_4^+ \text{ NH}_4^+ \text{ concentration in the soil liquid, g N kg}^{-1} \text{ soil} \]
\[ NH_4^+ \text{ NH}_4^+ \text{ concentration in liquid phase, mol L}^{-1} \]
\[ NH_4(t) \text{ available NH}_4^+ \text{ at time t, kg N ha}^{-1} \]
\[ N_2O \text{ daily emission of N}_2O, \text{ ng N m}^{-2} \text{ soil d}^{-1} \]
\[ pH \text{ soil pH.} \]
\[ R_0 \text{ total decomposed residue C, kg C} \]
\[ S \text{ labile fraction of organic C compounds in the pool.} \]
\[ t \text{ time, d.} \]
\[ P_{\text{comb}} \text{ combined temperature and moisture reduction factor.} \]
\[ P_{\text{CLAY}} \text{ clay content reduction factor} \]
\[ P_{\text{C:N}} \text{ C:N ratio reduction factor} \]
\[ P_{\text{m}} \text{ moisture reduction factor for nitrification.} \]
\[ P_{\text{t}} \text{ temperature reduction factor for nitrification.} \]

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