DNDC

(Version 9.5)

Scientific Basis and Processes

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DISCLAIMER

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1. Introduction

The Denitrification-Decomposition (DNDC) model is a process-based model of carbon (C) and nitrogen (N) biogeochemistry in agricultural ecosystems. This document describes general scientific basis and key processes of the DNDC model for predicting crop yield, soil environmental factors, C sequestration, and emissions of C and N gases in agro-ecosystems. Other contents regarding the DNDC model, including model installation, input and output, uncertainty analysis, andcase studies, can be found at User's Guide for the DNDC Model (http://www.dndc.sr.unh.edu/model/GuideDNDC95.pdf). Relevant publications of DNDC can be found at the DNDC website (http://www.dndc.sr.unh.edu/)or the Global DNDC Network (http://www.globaldndc.net/information/publications-i-3.html). These publications provide more information about the scientific basis, processes, and applications of DNDC far beyond this document.

2. DNDC Background

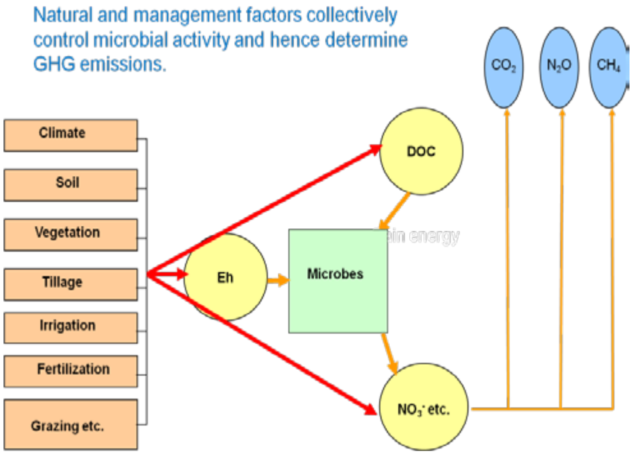

Fig. 1. DNDC functional overview. DNDC predicts GHG emissions based on activations of functional groups of microbes driven by E_h, DOC and oxidant concentration in the environment. Climate, soil properties and management practices collectively drive soil E_h, DOC and oxidant concentrations and hence determine the microbial functions to produce CO_2, N_2O or CH_4.

The DNDC model (Li et al., 1992a, 1992b, 1994, 1996; Li, 2000) was developed for quantifying C sequestration and emissions of greenhouse gases (GHG), and has been extensively evaluated against datasets of trace gases fluxes that were measured worldwide (e.g., Gilhespyet al., 2014; Giltrap et al., 2010). The core of DNDC trace-gas emission predictions consists of microbe-mediated biogeochemical processes commonly occurring in terrestrial soils. The processes primarily include decomposition, nitrification, denitrification, fermentation, and methanogenesis. DNDC simulates rates of the processes by tracking activities of different groups of microbes which are activated under different environmental conditions including temperature, moisture, pH, redox potential (E_h) and substrate concentration gradient in soils. Nitrification is modeled as first order of soil ammonium (NH_4^+) concentration under aerobic conditions and (nitrous oxide) N_2O production in nitrification is modeled as a fraction of the nitrification rate. Denitrification induced N_2O production is initiated once soil is saturated, which is assumed to lead to relative anaerobic conditions suitable for denitrification. Soil E_h is calculated with the Nernst equation at a daily time step following soil saturation and then used to determine anaerobic microbial group activity under a given set of soil conditions. Anaerobic microbial group activity is then modeled using standard Michaelis-Menten-type kinetics.

The hypotheses backing the DNDC simulations of soil GHG currently include: a) carbon dioxide (CO_2), N_2O and methane (CH_4) are products of oxidation-reduction reactions through electron exchange between electron donors and acceptors that is mediated by microbes; b) the occurrence of the electron exchange is determined by the soil E_h that is described by the Nernst Equation, a thermodynamic equation calculating E_h based on the concentrations of paired oxidative and reductive forms of dominant oxidants in the soil; c) when the suitable E_h is established, the functional group of bacteria will grow to their full capacity within a short timeframe (hours or days) due to rapid regeneration; and d) when the microbial capacity is established, the reaction rate will be primarily controlled by the concentrations of the relevant substrates based on the Michaelis-Menten Equation. DNDC currently tracks microbial activity primarily based on three drivers, i.e., E_h, dissolved organic carbon (DOC) as electron donor, and oxidants (such as oxygen, nitrate, and CO_2) as electron acceptors. Figure 1 provides a functional overview of DNDC and how natural factors and management practices influence Eh, DOC, substrate concentrations, and GHG emissions. Note that a secondary source of N_2O in the soil under aerobic conditions may be nitrifiers, which use NH_4^+ or ammonia(NH_3) as an energy source and CO_2 as a carbon source. Nitrification-induced N_2O production is simulated by DNDC with NH_4^+ and NH_3 levels under aerobic conditions as a major driver.

3. DNDC Modeling Framework

The production and consumption of CO_2, N_2O, CH_4 or NH_3 from agriculture result from a series of biogeochemical reactions, which are directly or indirectly related to microbial activities in soils. These reactions primarily include hydrolysis, decomposition, nitrification, denitrification, ammonia volatilization, fermentation, methanogenesis etc. Most of the processes have been documented in various publications and can be incorporated into process-based models through proper parameterization. Overthe past twenty-five years, these biogeochemical reactions have been incorporated into the process-based biogeochemical DNDC model. DNDC stands for DeNitrification and DeComposition, two processes dominating N and C losses from soils into the atmosphere. The DNDC model has been intensively and independently tested by a wide range of researches worldwide with encouraging results (e.g., Gilhespy et al., 2014; Giltrap et al., 2010). The DNDC model has also been widely utilized for inventory and mitigation of GHG in North America, Europe, Asia and Oceania.

DNDC consists of two components (Figure 2). The first component, consisting of the soil climate, crop growth and decomposition sub-models, predicts soil temperature, moisture, pH, Eh, and substrate concentration profiles (e.g. ammonium, nitrate, DOC) based on ecological drivers (e.g., climate, soil, vegetation and anthropogenic activity). The second component, consisting of the nitrification, denitrification and fermentation sub-models, predicts C and N gases fluxes, such as nitric oxide (NO), N_2O, CH_4 and NH_3 fluxes, based on the soil environmental variables. The model has incorporated classical laws of physics, chemistry and biology, as well as empirical equations generated from laboratory studies, to parameterize each specific geochemical or biochemical reaction. The entire model forms a bridge between the C and N biogeochemical cycles and the primary ecological drivers. The details of the biogeochemical processes in DNDC are described as follows.

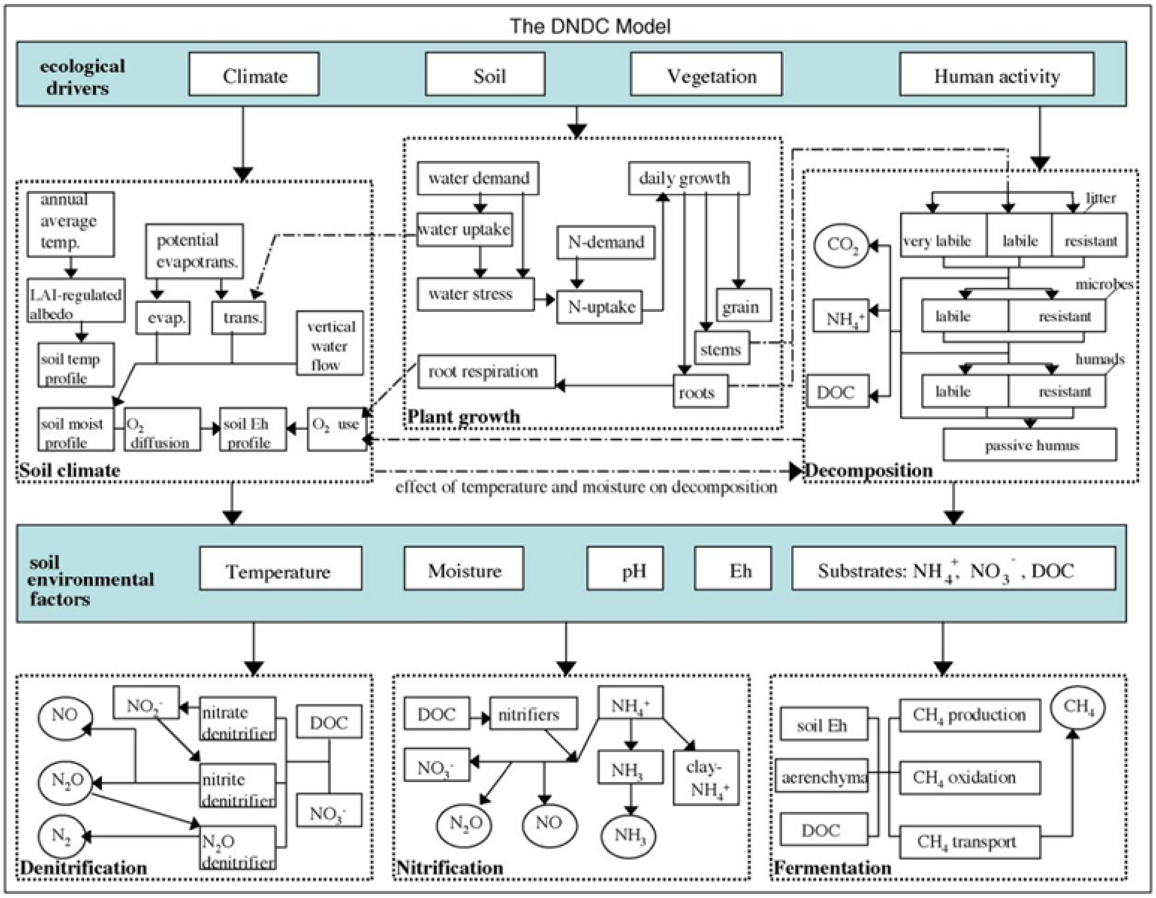

Figure 2 DNDC framework. The model consists of two components to link the ecological drivers, the soil environmental factors and the biogeochemical reactions including decomposition, nitrification, denitrification, fermentation, methanogenesis etc.

4. Modeling Redox Potential Dynamic and Soil Biogeochemistry under Aerobic and Anaerobic Conditions

Following rainfall events, irrigation, or flooding, soils can shift from unsaturated to saturated conditions, causing soil oxygen (O_2) depletion and resulting with more oxidants involved into the reductive reactions. These reductive reactions usually include denitrification of nitrate (NO_3^-), reductions of manganese (Mn^{4+}), iron (Fe^{3+}) and sulfate (SO_4^{2-}), and methanogenesis. These reductive reactions are driven by the soil microbial activities, which consume DOC or other C sources and pass electrons to the oxidants to obtain energy. Since different oxidants possess different Gibbs free energies, they accept electrons only under certain redox potential (i.e., Eh) conditions. Based on the Nernst equation (Eq. 1), soil Eh is determined by concentrations of the existing oxidants and reductants in the soil liquid phase (Stumm and Morgan, 1981).

Nernst equation: $Eh = E_0 + RT/nF \bullet \ln([\text{oxidant}]/[\text{reductant}])$ [Eq. 1]

where Eh is redox potential of an oxidation-reduction system (V), E_0 is standard electromotive force (V), R is the gas constant (8.314 J/mol/k), T is absolute temperature (273 + t, ºC), n is transferred electron number, F is the Faraday constant (96,485 C/mol), [oxidant] is concentration (mol/l) of dominant oxidant in the system, and [reductant] is concentration (mol/l) of dominant reductant in the system.

Under anaerobic conditions, the consumption of oxidants due to the microbial activity gradually decreases soil Eh. The consumption rates of the oxidants can be described by the Michaelis-Menten equation (Eq. 2). Based on the dual-nutrient Michaelis-Menten equation, rate of each reaction is controlled by the oxidant content and available C concentration (Paul and Clark, 1989):

$$F_{[\text{oxidant}]} = a\,[DOC / (b + DOC)] * [\text{oxidant} / (c + \text{oxidant})] \quad \text{[Eq. 2]}$$

where $F_{[\text{oxidant}]}$ is fraction of the oxidant reduced during a time step, DOC is concentration of DOC, oxidant is concentration of dominant oxidant in the oxidation-reduction system, and a, b and c are coefficients.

Since the Nernst and Michaelis-Menten equations share a common factor (i.e., oxidant concentration), a simple kinetic scheme was adopted in DNDC that links the two equations based on oxidant concentration. The kinetic scheme is defined to be the anaerobic volumetric fraction of the soil. Based on concentrations of the dominant oxidants and reductants in the soil, the Nernst equation calculates the soil bulk Eh. Based on the Eh value, the soil is divided into two parts: relatively anaerobic micro-sites (within the anaerobic volumetric fraction) and relatively aerobic micro-sites (outside of the anaerobic volumetric fraction). Based on these proportions, DNDC allocates the substrates (e.g., DOC, NO_3^-, NH_4^+, etc.) into the soil aerobic and anaerobic micro-sites. Substrates within the anaerobic volumetric fraction are subjected to the reductive reactions (e.g., denitrification, methanogenesis etc.); and substrates allocated outside of the anaerobic volumetric fraction are subjected to the oxidation reactions (e.g., nitrification, methanotrophy etc.). The Michaelis-Menten equation is used to determine the rates of the reactions occurring within and outside of the anaerobic volumetric fraction. Since the anaerobic volumetric fraction in soils is dynamic, DNDC quantifies this effect as an "anaerobic balloon", which swells or shrinks driven by the reduction/oxidation reactions (Figure 3). When a soil is irrigated or flooded, oxygen content will decrease, causing the anaerobic balloon to swell (i.e., the anaerobic volumetric fraction to increase). As soon as the oxygen is depleted, the anaerobic balloon will reach its maximum and burst. At this moment, a new oxidant (i.e., NO_3^-) will become the dominant species in the soil; and a new anaerobic balloon will be born and swell driven by the NO_3^- depletion. By tracking the formation and deflation of a series of anaerobic balloons driven by depletion of oxygen, NO_3^-, Mn^{4+}, Fe^{3+}, SO_4^{2-}, and CO_2, DNDC estimates soil Eh dynamics as well as production and consumption of the products from the reductive/oxidative reactions, including CO_2, N_2O and CH_4 (Figure 3). With the anaerobic balloon concept, DNDC links soil Eh dynamics with substrate concentrations and trace gas emissions from soils (Li et al., 2004).

An "anaerobic balloon" integrating Eh with redox reactions

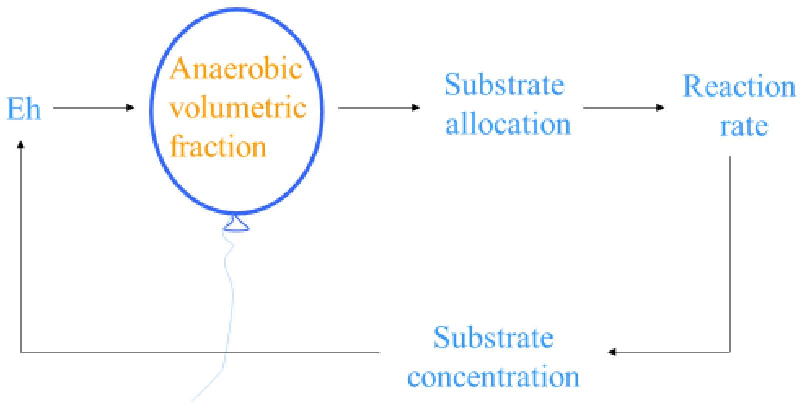

Figure 3 DNDC model's "Anaerobic Balloon" concept for tracking processes under aerobic and anaerobic conditions simultaneously.

DNDC's ability to simultaneously model nitrification and denitrification (Figure 4) by tracking anaerobic volume fraction is a key feature that allows the model to simulate N_2O fluxes across a broad range of soil environmental conditions and microbial mediated pathways.

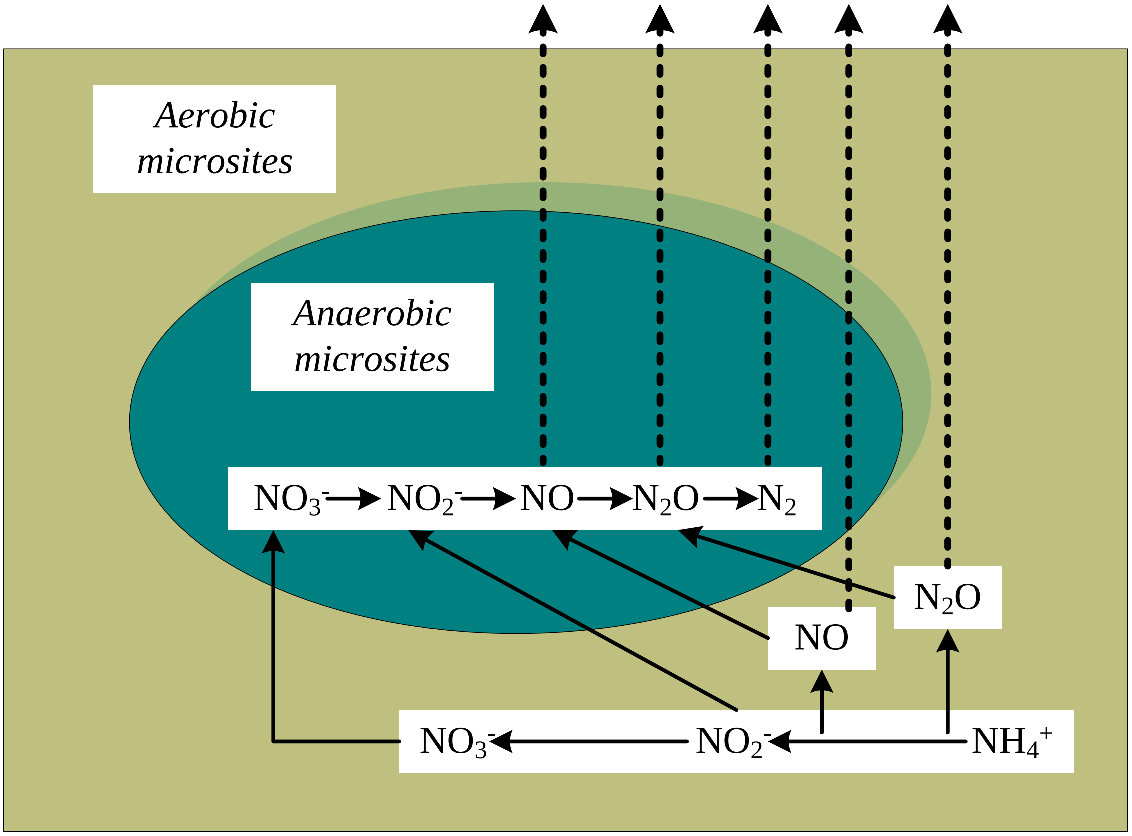

Figure 4 DNDC tracks fraction of soil aerobic and anaerobic micro-sites and nitrification and denitrification processes, which dominate N_2O production and consumption.

5. DNDC Processes

In this section, we discuss DNDC processes that simulate C and N cycling, production and consumption of GHGs, and ammonia volatilization. Processes of decomposition, urea hydrolysis, NH_3 production and emission, and NH_3 absorption by plants are described in Table 1 and key equations involving N_2O productions through nitrification and denitrification are provided in Table 2 and Table 3, respectively. Discussions on individual processes are in the following.

Table 1. Processes of decomposition, urea hydrolysis, NH_3 production and emission, and NH_3 absorption by plants simulated in DNDC.

Process 1. Decomposition rate of organic carbon pool

$dC/dt = CNR * \mu * (S * k_l + (1\text{-}S) * k_r) * [C]$ [Eq. 3]

Where [C] is organic C content (kg C/ha), t is time (day), S is labile fraction of organic C compounds in the pool, (1-S) is resistant fraction of organic C compounds, k_l is specific decomposition rate (SDR) of labile fraction (1/day), k_r is SDR of the resistant fraction (1/day), μ is temperature and moisture factor, CNR is C/N ratio reduction factor, SDR is 0.074, 0.074, 0.02, 0.33, 0.04, 0.16 and 0.006 (1/day) for very labile litter, labile litter, resistant litter, labile microbes, resistant microbes, labile humads, and resistant humads, respectively.

Process 2. Urease activity

$UREASE = k1 * [DOC] * WFPS * T$ [Eq. 4]

Where UREASE is urease activity (percent of urea hydrolyzed per day), [DOC] is dissolved organic carbon content (kg C/ha), WFPS is water-filled porosity, T is temperature (^oC), and k1 is a coefficient.

Process 3. Urea hydrolysis

$dUrea = [Urea] * UREASE$ [Eq. 5]

Where dUrea is daily hydrolyzed urea which is totally converted into NH_4^+, and [Urea] is concentration of urea (kg N/ha).

Process 4. NH_4^+/NH_3 equilibrium

$NH_4^+ = NH_3 + H^+$ [Eq. 6]

$Ka = [NH_4^+][OH^-] / [NH_3(l)]$ [Eq. 7]

$[H^+] = 10^{-pH}$ [Eq. 8]

$H_2O = H^+ + OH^-$ [Eq. 9]

$Kw = [H^+][OH^-]$ [Eq. 10]

$Ka = (1.416 + 0.01357 * T) * 10^{-5}$ [Eq. 11]

$Kw = 10\text{^}(0.08946 + 0.03605 * T) * 10^{-15}$ [Eq. 12]

Where Ka is equilibrium constant, Kw is water dissociation constant, $[NH_4^+]$, $[OH^-]$

and $[NH_3(l)]$ are NH_4^+, OH^- and $NH_3(l)$ concentrations (mol/l) in soil water, pH is soil pH, T is soil temperature.

Process 5a. NH_3 diffusion from the bulk liquid to the interface liquid phase

$Fl = Kl * ([NH_3]_{bl} - [NH_3]_{il})$ [Eq. 13]

where Fl is NH_3 diffusion rate in liquid phase (kg N/m^2/hr), Kl is NH_3 mass transfer coefficient in the liquid boundary layer, $[NH_3]_{bl}$ is NH_3 concentration in the bulk liquid phase (kg N/m^3), $[NH_3]_{il}$ is NH_3 concentration in the interface liquid phase (kg N/m^3).

Process 5b. NH_3 transfer from the interface of liquid phase to the bulk air

$Fg = Kg * ([NH_3]_{ig} - [NH_3]_{ag})$ [Eq. 14]

Where Fg is NH_3 transfer rate from the interface of liquid phase to the bulk air (kg N/m^2/hr), Kg is NH_3 mass transfer coefficient in the air boundary layer, $[NH_3]_{ig}$ is NH_3 concentration in the interface gas phase (kg N/m^3), $[NH_3]_{ag}$ is NH_3 concentration in the air (kg N/m^3).

Process 5c. Equilibrium between NH_3 in the interface of liquid and NH_3 in the interface of gas phase

$[NH_3]_{ig} = Kh * [NH_3]_{il}$ [Eq. 15]

Where $[NH_3]_{ig}$ is NH_3 concentration in the interface of gas phase (kg N/m^3), $[NH_3]_{il}$ is NH_3 concentration in the interface of liquid phase (kg N/m^3), Kh is Henry's coefficient.

Process 6a. NH_4^+ adsorption by clay

$FIXNH_4 = (0.41 - 0.47 * \log([NH_4])) * (CLAY/CLAY_{max})$ [Eq. 16]

Where $FIXNH_4$ is proportion of adsorbed NH_4^+, $[NH_4]$ is NH_4^+ concentration in the soil liquid (g N/kg), CLAY is clay fraction in soil, $CLAY_{max}$ is maximum clay fraction (0.63).

Process 6b. NH_3 absorption by plants in field

$PlantUp\_NH_3 = Vg * Air\_NH_3 * LAI * 0.864$ [Eq. 17]

$Vg = MaxVg * F(plant\text{-}N) * F(lsm)$ [Eq. 18]

$F(plant\text{-}N) = Plant\text{-}N(act) / Plant\text{-}N(opt)$ [Eq. 19]

$F(lsm) = LSM(act) / LSM(max)$ [Eq. 20]

$Air\_NH_3 = Base\_NH_3 + Flux\_NH_3 * 10\text{^}9 / V(canopy)$

$*LAI / (LAI + k2) * k3$ [Eq. 21]

Where $PlantUp\_NH_3$ is daily NH_3 absorption by plant, Vg is NH_3 deposition velocity (m/s), MaxVg is maximum velocity (0.050 m/s), Plant-N(act) is N content (kg N/ha) in crop, Plant-N(opt) is optimum N content (kg N/ha) in crop, LSM(act) is water content on leaf surface (cm), LSM(max) is maximum water content on leaf surface (cm), $Base\_NH_3$ is atmospheric background NH_3 concentration (μg/m3), $Flux\_NH_3$ is daily

NH_3 flux (kg N/ha) from soil, V(canopy) is volume of the room from ground to the top of canopy (m^3), LAI is leaf area index, and k2 and k3 are coefficients.

5.1. Decomposition

Decomposition is a process describing degradation of the organic matter. Since decomposition is mediated by the microbes living in the soil, part of the soil organic carbon (SOC) will be used as energy source resulting in CO_2 production, and another part of the SOC used for the microbial construction. During the decomposition, labile C will be gradually lost with resistant C become relatively more abundant in the soil. DNDC simulates SOC decomposition by simultaneously calculating the decomposition rate for each of the SOC sub-pools (i.e., litter, microbes, humads and passive humus). Figure 5 shows the sequential decomposition processes parameterized in DNDC, which convert litter to microbial biomass, humads, and finally humus. During the decomposition process, each sub-pool decomposes independently via first-order kinetics (see Process 1 in Table 1). As a microbe-mediated process, decomposition rate is subject to temperature and moisture. Decomposition rate will decline if the environmental temperature or moisture deviates from the optimum. The formulations have been widely used to estimate mineralization potentials of soil organic carbon, and yield results consistent with data from incubation studies (Molina et al., 1983; Stanford and Smith, 1972; Smith et al., 1980; Deans et al., 1983; El-Haris et al., 1983; Deans et al., 1986). Since aerobic decomposition requires oxygen as electron acceptor, improvement of soil aeration will accelerate the decomposition rate. However, decomposition can also take place under anaerobic conditions where hydrolysis degrades carbohydrates, proteins, celluloses and even lignin, especially in company with high temperature or catalyzing microbes. During the SOC decomposition process, the organic N that is contained in the soil organic matter is mineralized to ammonium, an inorganic ion that is not only an essential nutrient for almost all the plants or microbes but the sole precursor for other inorganic N species (e.g., nitrate and ammonia) commonly found in the soil.

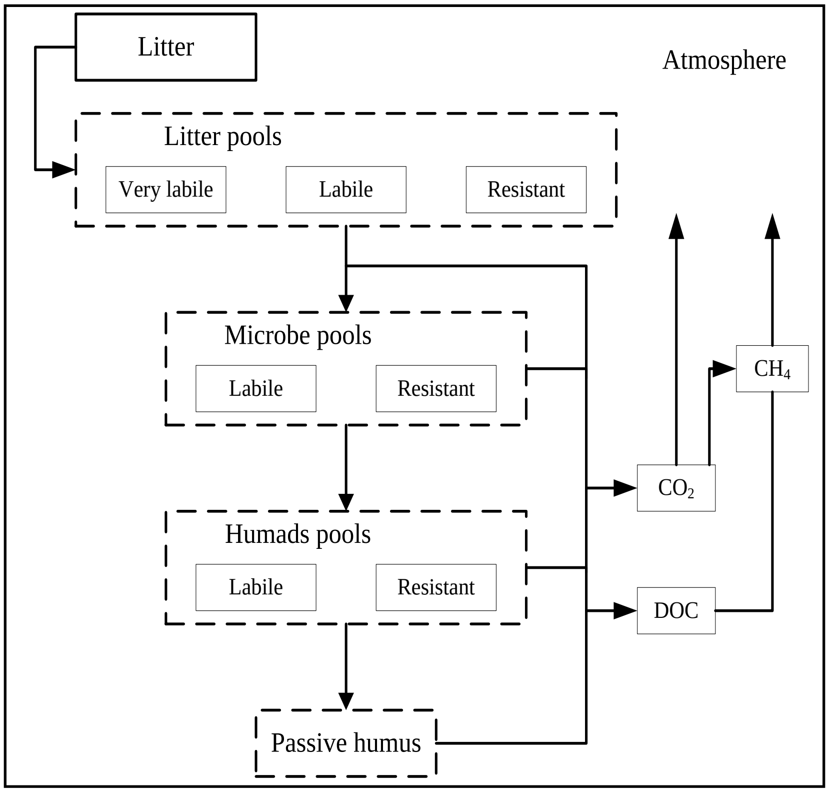

Figure 5. SOC pools and decomposition processes in DNDC.

5.2. Urea hydrolysis

Hydrolysis converts urea into ammonium. Hydrolysis is a chemical reaction during which water molecules are split into hydrogen and hydroxide ions which can further react with organic molecules such as urea ($CO(NH_2)_2$). During the hydrolysis, a molecule of urea is converted to two molecules of ammonium (NH_4^+) with a hydroxyl (OH^-) released (Eq. 22).

$$CO(NH_2)_2 + 3H_2O = 2NH_4^+ + HCO_3^- + OH^- \qquad [Eq.\ 22]$$

Hydrolysis of urea is catalyzed by urease, an enzyme whose activity is subject to temperature, moisture, and available organic carbon components. In DNDC, the urease activity in soil is calculated as a linear function of temperature, moisture and DOC content; and urea hydrolysis rate is the product of the urease activity and urea concentration (see Processes 2 and 3 in Table 1). Urea hydrolysis occurs in the soil whenever the substrates are available and temperature is favorable. The hydroxyl released from the urea hydrolysis elevates the soil pH which in turns affects a series of biogeochemical processes including NH_3 volatilization.

5.3. Ammonia volatilization

When ammonium (NH_4^+) is applied through fertilization or produced from either decomposition or urea hydrolysis, the NH_4^+ dissolved in the liquid will keep in equilibrium with the dissolved ammonia (NH_3) (Eq. 23).

$$NH_4^+ = NH_3^{\uparrow} + H^+ \qquad \text{[Eq. 23]}$$

The reaction can shift in either direction depending on the NH_4^+concentration, NH_3 concentration and pH in the liquid phase. To calculate the reaction rate, two dissociation constants for the NH_4^+/NH_3 equilibrium (Ka) and the H^+/OH^- equilibrium (Kw) are utilized. As Ka and Kw are temperature-dependent, DNDC calculates Ka and Kw as functions of temperature (Process 4 in Table 1) following Glasstone (1946) and Sutton et al. (1993). As soon as NH_3 is formed, it can diffuse to the liquid/air interface driven by the NH_3 concentration gradients. A two-film module has been adopted in DNDC to quantify the NH_3 emissions from the surface of soils. Following De Visscher et al. (2002), the Henry's law and NH_3 mass transfer coefficients were utilized to construct the two-film module in DNDC (Process 5a,b, and c in Table 1). DNDC uses the Langmuir equation to quantify adsorption and desorption of ammonium ions on clay and organic matter (OM). Ammonium adsorption is modeled as logarithmic relationship between ammonium concentration and clay fraction in the soils. Ammonia can be absorbed by crops/vegetation. DNDC models ammonia adsorption on crops based on daily ammonia flux and biophysical conditions of the crop (LAI, plant heights, and leaf moisture). Process 6a and b in Table 1 describe ammonium adsorption and ammonia adsorption by crops, respectively.

5.4. Nitrification

Under aerobic conditions, NH_4^+ can be oxidized to NO_2^- and further to NO_3^- by ammonium oxidizers (Eq. 24) (McGill et al., 1981; Van Veen and Frissel, 1979). This two-step process is called nitrification. During nitrification, a certain amount of NO or N_2O can be evolved as a byproduct (Bremner and Blackmer, 1978; Parton et al., 1988).

$$NH_4^+ + O_2 \rightarrow NO_2^- + 4H^+ + 2e^-$$
$$NO_2^- + H_2O \rightarrow NO_3^- + 2H^+ + 2e^-$$ [Eq. 24]

As a microbe-mediate process, the rate of nitrification is regulated by soil temperature, moisture, Eh and pH (Watts and Hanks 1978; Hadas et al., 1986) and nitrifiers' activity, which relies on two substrates, DOC and NH_4^+. In DNDC, the growth and death rates of nitrifiers are set as functions of DOC and soil moisture (Equations 25 to 27 in Table 2) based on Blagodatsky and Richter (1998). The reaction rate of nitrification is subject to nitrifiers' activity as well as other environmental factors such as NH_4^+ availability and pH (Eq. 28 in Table 2). Based on Bremner and Blackmer (1981), the nitrification-derived N_2O is a fraction of the nitrification rate (Eq. 31 in Table 2).

Table 2. Key equations for simulating N_2O production through nitrification.

Relative growth (dG/dt) and death rates (dD/dt) of nitrifiers

$$dG/dt = 0.0166*([DOC]/(1.0+[DOC]) + Fm/(1.0+Fm))$$ [Eq. 25]

$$dD/dt = 0.008*Nitrifier*1.0/(1.0+[DOC])/(1.0+Fm)$$ [Eq. 26]

Where [DOC] is dissolved organic carbon content (kg C/ha), Fm is a soil moisture factor, and Nitrifier is biomass of nitrifier.

Net increase in nitrifier biomass

$$dNitrifier/dt = (dG/dt - dD/dt)*Nitrifier*Ft*Fm$$ [Eq. 27]

Nitrification rate

$$RN = 0.005*[NH_4^+]*Nitrifier*pH$$ [Eq. 28]

Where $[NH_4^+]$ is concentration of ammonium (kg N/ha) and pH is the soil pH.

Soil moisture factor in nitrification

$$Fm = 0.8 + 0.21*(1.0 - WFPS) \quad WFPS > 0.05$$
$$Fm = 0.0 \quad WFPS \le 0.05$$ [Eq. 29]

Where WFPS is the soil water content in water filled porosity.

Soil temperature factor in nitrification

$$Ft = 3.503^{((60-T)/25.78)} * \exp^{(3.503*(T-34.22)/25.78)} \qquad \text{[Eq. 30]}$$

Where T is the soil temperature.

N_2O production through nitrification

$$N_2O_N = 0.0024 * RN \qquad \text{[Eq. 31]}$$

Where RN is the nitrification rate as in Eq. 28.

5.5. Denitrification

Denitrification is a series of microbe-mediated reactions that sequentially reduce nitrate (NO_3^-) to nitrite (NO_2^-), nitric oxide (NO), nitrous oxide (N_2O), and finally dinitrogen (N_2) (Eq. 32). As reductive reactions, the denitrifying sequence can occur only under anaerobic conditions.

$$NO_3^- + 2e^- \rightarrow NO_2^- + e^- \rightarrow NO + e^- \rightarrow N_2O + 2e^- \rightarrow N_2 \qquad \text{[Eq. 32]}$$

Leffelaar and Wessel (1988) presented a detailed description of denitrification processes based on lab incubations with soil samples. They observed that the rate of each step of the sequential reactions depended on the concentration of the corresponding nitrogenous oxides (i.e., NO_3^-, NO_2^-, NO, or N_2O), and all the reactions competed for available C (i.e., DOC). These relationships were applied in DNDC to form the denitrification algorithms. In DNDC, the denitrifying conditions are assumed if the environmental Eh drops to 500 mV or lower due to the oxygen depletion in the soil, and denitrification occurs in soil anaerobic micro-sites, whose volumetric fractions are defined by the “anaerobic balloon” embedded in the DNDC framework (see the section of "Modeling redox potential dynamic and soil biogeochemistry under aerobic and anaerobic conditions"). In DNDC, all denitrifiers are capable of anaerobic growth only in the presence of DOC and nitrogenous oxides (i.e., NO_3^-, NO_2^-, NO, or N_2O). The denitrifiers grow by consuming the corresponding N oxides. The growth rates of the denitrifying bacteria are assumed to be proportional to their respective amounts of biomass (van Veen and Frissel, 1979; Equations 33 to 35 in Table 3). Relative growth rates, which depend on the concentrations of DOC and the corresponding electron acceptors (i.e., N-oxides), can be calculated with the dual-Monod kinetics, a simple function describing multiple-nutrient-dependent Michaelis-Menten type growth (Bader, 1978). Following Leffelaar and Wessel (1988), the model assumes that the relative growth rates for denitrifiers with different substrates are independent; competition among the bacteria takes place via the common soluble C substrate (Equations 33 and 34 in Table 3). The denitrifier death rate is modeled as proportional to denitrifier biomass (Eq. 36 in Table 3). The C and N from dead cells are added to the pools of immobilized C and N pools (i.e., humads) and no longer participate in the dynamic processes (Leffelaar and Wessel, 1988).

The effects of soil pH or temperature on denitrification are modeled in DNDC based on observations reported by a number of studies (Mueller et al., 1980; Klemedtsoon et al., 1978; Burford and Bremner, 1975; Stanford et al., 1975a; Khan and Moore, 1968; Wijler and Delwiche, 1954; Focht, 1974; Leffelaar and Wessel, 1988; Nommik, 1956; Dawson and Murphy, 1972; Bailey and Beauchamp, 1973; Stanford et al., 1975b; Knowles, 1981; Keeney et al., 1979; Bremner and Shaw, 1958) (Equations 41 and 42 in Table 3). DOC is used by denitrifiers as the basic material for cell synthesis and energy (Pirt, 1965). The consumption rate of DOC depends on the denitrifier biomass, relative growth rate, and maintenance coefficients of the denitrifier populations (Eq. 37 in Table 3). CO_2 production is calculated as the difference between the total amount of consumed C and the amount used for cell synthesis (Eq. 38 in Table 3). NO_3^-, NO_2^-, and N_2O consumptions are calculated with Pirt's equation. According to Leffelaar and Wessel (1988), the maintenance coefficients must be multiplied by the relative presence of each electron acceptor in the water phase, because maintenance data reported in the literature for each reducing step are for maintenance sufficient to support the entire denitrifier biomass (NO_3^-denitrifier + NO_2^-denitrifier + N_2O denitrifier) (Eq. 39 in Table 3). Based on the growth rates of denitrifiers and the C/N ratio in the bacteria, the assimilation of N during denitrification is calculated (Eq. 40 in Table 3). A C/N ratio (by weight) of 3.45 is used based on the chemical composition of denitrifiers ($C_6H_{10.8}N_{1.5}O_{2.9}$), in accordance with data reported for *Paracoccus denitrificans* (Verseveld and Stouthamer, 1978).

Table 3. Key equations for simulating N_2O production through denitrification.

Relative growth rates of NO_X denitrifiers

$$u_{NOx} = u_{NOx,max} * \left([DOC] / \left(K_C + [DOC] \right) \right) * \left([NOx] / \left(K_N + [NOx] \right) \right) \qquad \text{[Eq. 33]}$$

$$u_{DN} = F_T * (u_{NO3} * F_{PH-NO3} + u_{NO2} * F_{PH-NO2} + u_{NO} * F_{PH-NO} + u_{N2O} * F_{PH-N2O}) \qquad \text{[Eq. 34]}$$

$$\left(dDenitrifier / dt \right)_g = u_{DN} * Denitrifier \qquad \text{[Eq. 35]}$$

Where $u_{NOx,max}$ is the maximum growth rate of NO_3^-, NO_2^-, NO, or N_2O denitrifiers, DOC is dissolved organic carbon content (kg C/ha), NOx is concentration of NO_3^-, NO_2^-, NO, or N_2O in soil water (kg N/ha), K_C is half-saturation value of soluble C in the Monod model (kg C/m^3 soil water), K_N is half-saturation value of NO_3^-, NO_2^-, NO, or N_2O in the Monod model (kg N/m^3 soil water), F_T is a temperature factor, F_{PH-NO3}, F_{PH-NO2}, F_{PH-NO}, and F_{PH-N2O} is soil pH factors, and Denitrifier is biomass of denitrifier.

Relative death rates of denitrifiers

$$\left(dDenitrifier / dt \right)_d = M_C * Y_C * Denitrifier \qquad \text{[Eq. 36]}$$

Where M_C is maintenance coefficient of C (kg C/kg C/hr) and Y_C is maximum growth yield on soluble carbon (kg C/kg C).

Consumption of DOC and CO_2 production through denitrification

$$dC_{con} / dt = \left(u_{DN} / Y_C + M_C \right) * Denitrifier \qquad \text{[Eq. 37]}$$

$$dCO_2 / dt = dC_{con} / dt - dDenitrifier / dt \qquad \text{[Eq. 38]}$$

Consumption of NO_X through denitrification

$$\begin{aligned} d\left(NO_3 \right) / dt &= (u_{NO3} / Y_{NO3} + M_{NO3} * [NO_3] / [N]) * Denitrifier * F_{PH-NO3} * F_T \\ d\left(NO_2 \right) / dt &= (u_{NO2} / Y_{NO2} + M_{NO2} * [NO_2] / [N]) * Denitrifier * F_{PH-NO2} * F_T \\ d\left(NO \right) / dt &= (u_{NO} / Y_{NO} + M_{NO} * [NO] / [N]) * Denitrifier * F_{PH-NO} * F_T \\ d\left(N_2O \right) / dt &= (u_{N2O} / Y_{N2O} + M_{N2O} * [N_2O] / [N]) * Denitrifier * F_{PH-N2O} * F_T \end{aligned} \qquad \text{[Eq. 39]}$$

Where Y_{NO3}, Y_{NO2}, Y_{NO}, and Y_{N2O} is the maximum growth yield on NO_3^-, NO_2^-, NO, or N_2O (kg C/kg N), M_{NO3}, M_{NO2},M_{NO},and M_{N2O} is the maintenance coefficient of NO_3^-, NO_2^-, NO, or N_2O (kg N/kg/hr), and N is the total nitrogen as the sum of NO_3^-, NO_2^-, NO, and N_2O (kg N/ha).

Assimilation of N during denitrification

$$dN / dt = (dDenitrifier / dt)_g / (C / N)_{Denitrifier} \qquad \text{[Eq. 40]}$$

Where C/N $_{\text{denitrifier}}$ is C/N ratio in denitrifiers.

Soil temperature factor in denitrification

$$F_T = 2.0^{(T-22.5)/10.0} \quad T \le 60.0$$
$$F_T = 0.0 \quad T > 60.0 \qquad \text{[Eq. 41]}$$

Where T is the soil temperature.

pH factor in denitrification

$$F_{PH-NO3} = 1 - 1/(1 + \exp^{((pH-4.25)\ /\ 0.5))}$$
$$F_{PH-NO2} = F_{PH-NO} = 1 - 1/(1\ +\ \exp^{((pH-5.25)/1))} \qquad \text{[Eq. 42]}$$
$$F_{PH-N2O} = 1 - 1/(1 + \exp^{((pH-6.25)\ /\ 1.5))}$$

Where pH is the soil pH.

5.6. Methane dynamics

The rate of methane emission is predicted by modeling its production, consumption, and transport processes (Figure 6). methane production is simulated by calculating substrate concentrations (i.e., electron donors and acceptors) resulting from decomposition of SOC as well as plant root activities including exudation and respiration, and then by tracking a series of reductive reactions between electron donors (i.e., H_2 and DOC) and acceptors (i.e., NO_3^-, Mn^{4+}, Fe^{3+}, SO_4^{2-}, and CO_2). The simulation of SOC decomposition hasbeen described at the section of "Decomposition". During decomposition of each SOC sub-pool, the model distributes a fixed fraction of the released C into DOC (Li et al., 1992a). DOC from SOC decomposition therefore depends on size and specific decomposition rate of each SOC pool, as well as soil thermal and moisture conditions (Li et al., 1992a, 2012). When a soil is shifting from unsaturated to saturated conditions, soil oxygen is gradually depleted and additional oxidants (e.g., NO_3^-, Mn^{4+}, Fe^{3+}, SO_4^{2-}, and CO_2) may become involved in reductive reactions. Soil Eh gradually decreases along with the consumption of these oxidants, and DNDC simulates denitrification, reductions of Mn^{4+}, Fe^{3+}, and SO_4^{2-}, and methane production as consecutive reactions with each reaction occurring under certain Eh conditions [Li et al., 2004]. DNDC simulates methane production after depletions of NO_3^-, Mn^{4+}, Fe^{3+}, and SO_4^{2-}, when soil Eh is below -150 mV (Li et al., 2004). Methane consumption is simulated as an oxidation reaction involving electron exchange between CH_4 and oxygen. In DNDC, CH_4 production and oxidation can occur simultaneously within a soil layer (around2 cm thick) but within relatively aerobic and anaerobic sub-layers, whose volumetric fractions are determined by Eh calculations (Li, 2007). Redox potential, temperature, pH, and the concentrations of electron donors and acceptors are the major factors controlling the rates of CH_4 production and oxidation. Methane transport from soil into atmosphere is simulated via three ways, including plant-mediated transport, ebullition, and diffusion (Fumoto et al., 2008; Zhang et al., 2003).

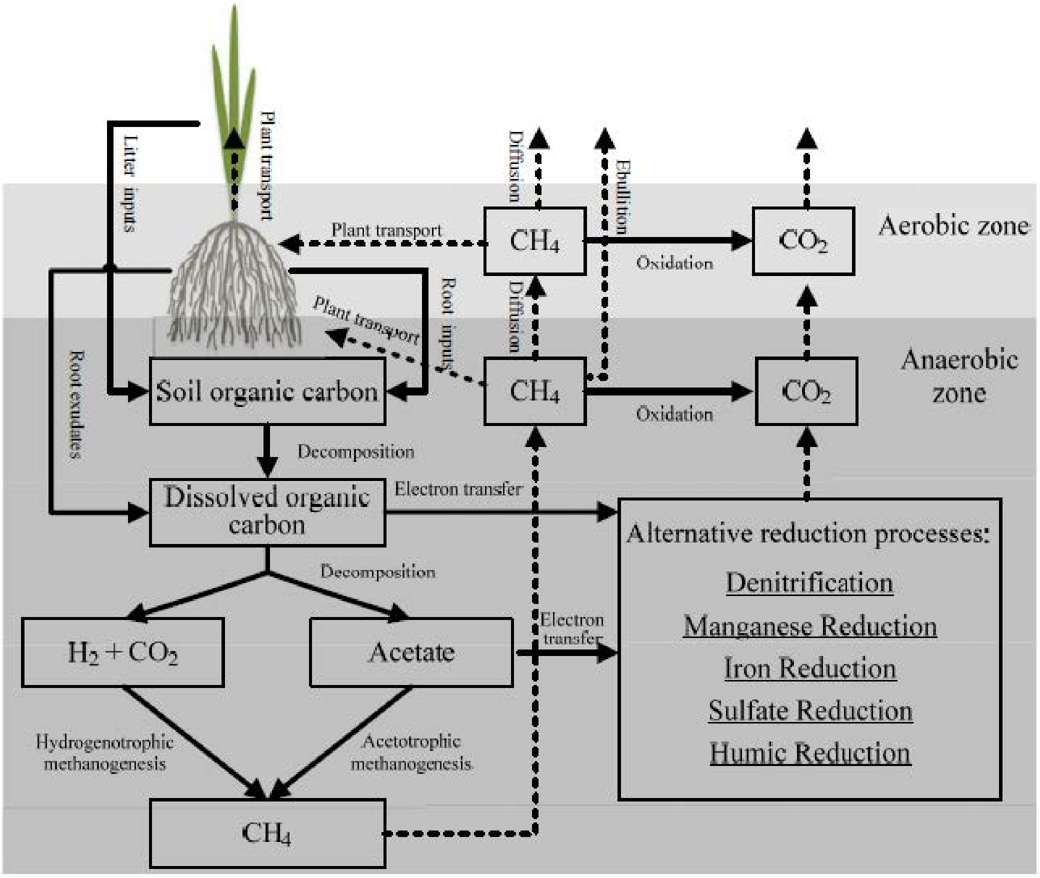

Figure 6 The framework for simulating soil biogeochemistry and methane dynamics in the modified DNDC.

6. Modeling Environmental Factors

All the biogeochemical reactions are controlled by a group of environmental factors such as temperature, moisture, pH, Eh and substrate concentration. These environmental factors form a biogeochemical field which collectively and simultaneously determines the occurrences and rates of the biogeochemical reactions in the soil (Figure 7). Most of the environmental factors vary in space and time driven by both natural conditions (e.g., climate, soil, vegetation etc.) and management activities (e.g., irrigation, tillage etc.). In DNDC, daily weather data (e.g., air temperature, precipitation and wind speed), soil properties (e.g., bulk density, texture, SOC content and pH), vegetation characteristics and field management activities are used as inputs to determine the dynamics of temperature, moisture, pH, Eh and substrate concentration in soil profile.

In DNDC, farming management practices (FMPs), such as tillage, fertilization, manure application, flooding, irrigation, and cultivation of cover crops, have been parameterized to regulate soil environmental conditions and/or substrate concentrations, and thereby can influence biophysical and biogeochemical reactions and their products. For example, N fertilization affects soil N pools based on N rate, method of application, and type of fertilizers, and therefore can affect crop growth, nitrate leaching, as well as emissions of C and N gases. Manure application incorporates manure into the soil.C and N bound in the organic manure is released through decomposition and distributed into the relevant soil C and N poolsand is then engaged in soil C and N cycling during the simulation. Flooding and irrigation directly control soil moisture and redox potential, which influence crop growth and all biogeochemical reactions. In DNDC, four irrigation methods, including surface irrigation, sprinkler, drip, and subsurface drip, have been parameterized. For different irrigation methods, water is allocated into different layers in the soil profile with different intensity. This setting has enabled the model to simulate the influence of irrigation methods on dynamics of soil redox potential and N_2O produced from nitrification and/or denitrification (Zhang et al., 2015).

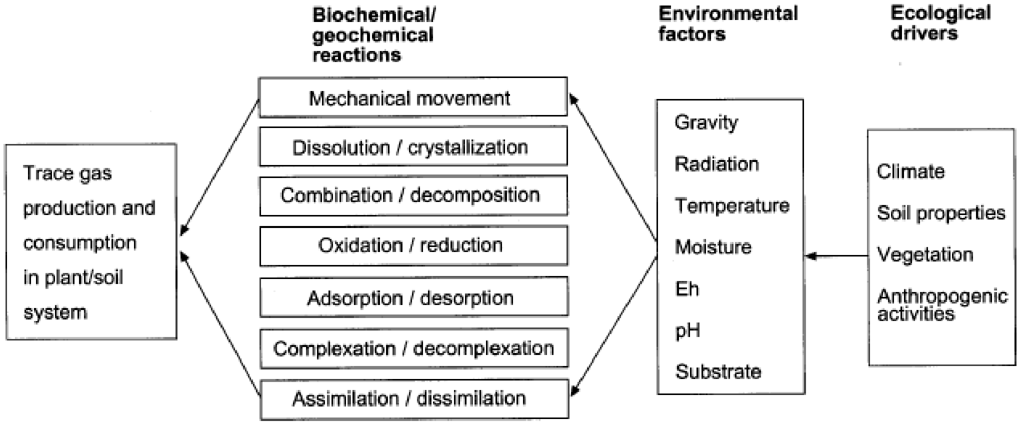

Figure 7 DNDC model links soil environmental factors with biogeochemical reactions to simulate production and consumption of trace gases in agricultural soils.

6.1. Soil temperature

Temperature is one of the most important factors affecting biochemical or geochemical reactions. In DNDC, soil temperature varies across different depth. The model calculates soil temperature based on heat transfer across the soil profile (Li et al. 1992a). The temperature of surface and deep soil, heat capacity and heat conductivity of each soil layer (about 2.0 cm) are calculated primarily based on air temperature and soil physical properties to determine the soil temperature profile at a daily time step.

6.2. Soil moisture

Water plays a dual role in soil biogeochemistry. Many biogeochemical reactions take place only in liquid phase and soil moisture is an important factor influencing soil redox potential. DNDC simulates soil moisture in each layer by calculating both surface and vertical water movements (Figure 8), including surface runoff, transpiration, evaporation, infiltration, water redistribution, and drainage (Deng et al., 2011; Li et al.,2006; Zhang et al., 2003). Primary factors influencing soil moisture include weather conditions (e.g., temperature, humidity, and wind speed), soil properties (e.g., texture, field capacity, wilt point, and hydrological conductivity, and previous soil water availability), crop growth, and FMPs (irrigation, flooding, film mulch etc.).

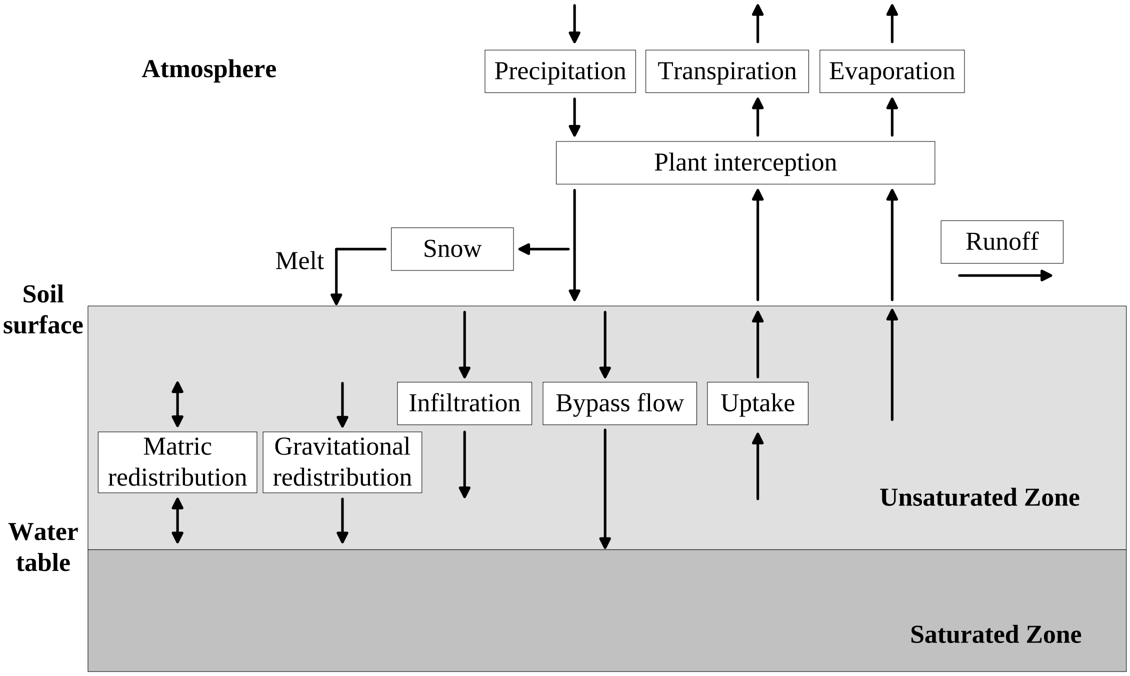

Figure 8 Structure of the soil hydrology submodel of DNDC. The solid arrows represent the processes existing in DNDC.

6.3. Soil Eh

The processes of decomposition, nitrification, denitrification or methanogenesis respectively producing CO_2, N_2O or CH_4 are typical reductive-oxidative reactions, which occur through electron exchange between the substrates. The environmental Eh determines the occurrence of the reactions based on the Gibbs free energy of formation (Stumm and Morgan, 1981). Under aerobic conditions, the Eh values in soils vary between 100-650 mV that is favorable for oxidative reactions such as decomposition, nitrification or methane oxidation. When the soil is saturated due to irrigation, flooding, or rainfall, oxygen in the soil will be depleted and lead to anaerobic conditions (Eh -300 to 0 mV), under which reductive reactions such as denitrifation or methanogenesis will occur. In reality, the aerobic and anaerobic micro-sites can simultaneously exit in a same soil layer although their volumetric proportions could vary according to the bulk Eh of the soil. DNDC approach for modeling Eh is provided in the section of "Modeling redox potential dynamic and soil biogeochemistry under aerobic and anaerobic conditions".

6.4. Soil pH

Environmental acidity represented as pH determines the proton (H^+) transferring capacity, which affects a wide range of soil biogeochemical reactions. For example, the hydrolysis of urea reduces the H^+ concentration in the soils, which in turn increases the soil pH. This increase in soil pH will lead to increases of NH_3 volatilization by shifting the NH_4^+/NH_3 equilibrium. DNDC tracks the variation of pH by counting H^+ production or consumption in the biogeochemical reactions at a daily time step. Urease activity, hydrolysis, NH_4^+/NH_3 equilibrium, NH_3 dynamics and NH_4^+ adsorption are discussed above.

6.5. Substrate concentration

DNDC simulates the biogeochemical reactions related to CO_2, CH_4, N_2O or NH_3 production and/or consumption based not only on the thermodynamic parameters (i.e., temperature, moisture, pH and Eh) but also the substrates concentrations, which determine the reaction kinetics of the biogeochemical processes. For microbe-mediated processes such as decomposition, nitrification, denitrification or fermentation, DOC is a common energy source. DNDC calculates DOC concentration in the soil as a balance between the DOC production from decomposition or plant exudation and the DOC consumption by heterotrophic bacteria (e.g., decomposers, nitrifiers, denitrifiers, methanogens, and methanotrophers) or leaching. For N biogeochemistry in soils, ammonium and nitrate play an active role in many processes such as nitrification, denitrification and ammonia volatilization. By tracking the N transport and transformations in the soils, DNDC calculates NH_4^+ and NO_3^- concentrations at a daily time step. NH_4^+ content increases due to decomposition and ammonification, and decreases due to nitrification, NH_3 volatilization, adsorption and plant uptake.NO_3^- content increases due to nitrification, and decreases due to denitrification, plant uptake and leaching. The modeled concentrations of DOC, NH_4^+ and NO_3^- are utilized to calculate the rates of the relevant biogeochemical processes as described above.

7. Modeling Crop Growth

In DNDC, crop biomass dynamicsare simulated at daily time step by considering the effects of several environmental factors on plant growth, including radiation, air temperature, and availability of soil water and N (Figure 9). The model calculates potential water and N demands for crop growth based on several physiological parameters, including the maximum biomass production and its partitioning fractions to shoot and root, the C/N ratio of plants, the accumulative temperature for maturity (TDD), water requirement, and the index of biological N fixation, and then predicts daily crop growth based on availability of soil water and mineral N. As Figure 9 illustrates, daily crop growth and yields are controlled by complex interactions of weather, soil conditions and crop physiological properties. Because crop growth affects soil water content, DOC, soil N pools, and production of plant litter that incorporated into SOC pools, it influences almost all the biogeochemical processes in DNDC through influencing soil environmental factors and/or substrates concentrations.

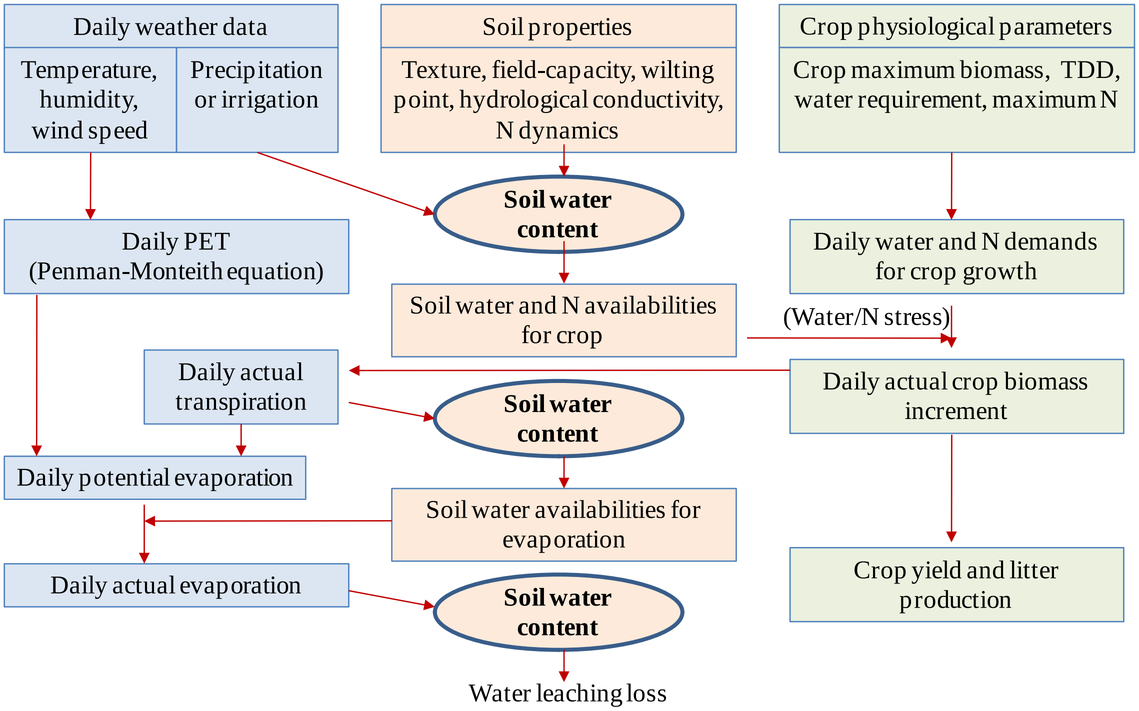

Figure 9 DNDC models interactions of weather, soil conditions and crop physiological properties for predicting daily crop growth and yields.

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