**DNDCv.CAN**

**Scientific Basis and Processes**

**A group of people working in a field

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## DISCLAIMER

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**1. Introduction**

The Denitrification-Decomposition (DNDC) model (Li et al., 1992a) is a process-based model of carbon (C) and nitrogen (N) biogeochemistry in agricultural ecosystems. The Canada DNDC model (DNDCv.CAN) is a version designed to better simulate soil-plant–climate interactions in cool weather climate (Smith et al., 2020). This document describes the general scientific basis and key processes of DNDCv.CAN for predicting crop growth and yield, soil environmental factors, C sequestration, and emissions of C and N gases in agricultural ecosystems. As DNDCv.CAN was modified from a base version of the DNDC model (DNDC version 95), some contents in this document are from the DNDC Scientific Basis and Processes (<https://www.dndc.sr.unh.edu/papers/DNDC_Scientific_Basis_and_Processes.pdf>). In addition, major developed or modified processes in DNDCv.CAN have been described in this document. Other contents regarding the DNDCv.CAN model, including model installation, input and output, model operation, uncertainty analysis, and case studies, can be found at User's Guides for the DNDC Model (<http://www.dndc.sr.unh.edu/model/GuideDNDC95.pdf>) and DNDCv.CAN model (<https://github.com/BrianBGrant/DNDCv.CAN/blob/master/DNDCvCAN%20User%20Guide.pdf>). Relevant publications of DNDC can be found at the DNDC website (<http://www.dndc.sr.unh.edu/>) and the Global DNDC Network (<https://globaldndc.net/publications>). These publications provide more information about the scientific basis, processes, and applications of the DNDC and DNDCv.CAN models.

**2. Background and Model Hypotheses**

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 C and N gases fluxes that were measured worldwide (e.g., Deng et al., 2014, 2020; Gilhespyet al., 2014; Giltrap et al., 2010). The core of DNDC trace gases emission predictions consists of microbe-mediated biogeochemical processes commonly occurring in terrestrial soils. The processes primarily include hydrolysis, decomposition, nitrification, denitrification, fermentation, and methanogenesis. DNDC simulates rates of these processes by tracking activities of different groups of microbes which are activated under different environmental conditions including temperature, moisture, pH, redox potential (Eh) and substrate concentration gradient in soils. Nitrification is modeled as the first order of soil ammonium (NH4+) concentration under aerobic conditions and nitrous oxide (N2O) and nitric oxide (NO) production in nitrification are modeled as fractions of the nitrification rate. Denitrification induced N2O production is initiated once soil is saturated, which is assumed to lead to relative anaerobic conditions suitable for denitrification. Soil Eh 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 Michaelis-Menten-type kinetics.

The hypotheses backing the DNDC simulations of soil GHG include: a) carbon dioxide (CO2), N2O and methane (CH4) are products of different 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 Eh that is described by the Nernst Equation, a thermodynamic equation calculating Eh based on the concentrations of paired oxidative and reductive forms of dominant oxidants in the soil; c) when the suitable Eh 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 tracks microbial activity primarily based on three drivers, i.e., Eh, dissolved organic carbon (DOC) as electron donor, and oxidants (such as oxygen, nitrate, and CO2) 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 N2O in the soil under aerobic conditions may be nitrifiers, which use NH4+ or ammonia (NH3) as an energy source and CO2 as a carbon source. Nitrification-induced N2O production is simulated by DNDC with NH4+ and NH3 contents under aerobic conditions as a major driver. The hypotheses and biogeochemical processes for simulating soil GHG emissions in DNDCv.CAN are the same as the DNDC model, although there are differences in simulating some processes and environmental variables.

A diagram of a microbial activity

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**Figure 1. DNDC functional overview.** DNDC predicts GHG emissions based on activations of functional groups of microbes driven by Eh, DOC and oxidant concentration in the environment. Climate, soil properties, vegetation, and management practices collectively drive soil Eh, DOC, and oxidant concentrations and hence determine the microbial functions to produce CO2, N2O, or CH4.

**3. Model Framework**

The production and consumption of CO2, N2O, CH4 or NH3 from agriculture soils 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. Over the past thirty years, these biogeochemical reactions have been incorporated into the process-based biogeochemical model DNDC to build the framework of the model. The framework of DNDCv.CAN is identical to the DNDC’s framework.

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 NO, N2O, CO2, CH4 and NH3 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 and/or field 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 and DNDCv.CAN are described as follows.



**Figure 2 Model 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. Model Operations**

The DNDCv.CAN model is a structured program that integrates numerous subroutines or functions to simulate relevant processes of cropping systems. The functions, relationships, and parameters used in these functions are described in detail in the following sections of this document. This section describes the linkage and flow of primary processes of the model (Figure 3).

The model begins by reading input information, primarily including site information, soil physical and chemical properties, crop characteristics, and farming management practices (FMPs) (planting and harvest, crop residue return, tillage, irrigation, fertilization, manure amendment etc.). All parameters gathered from model input interfaces and databases are read. Users can modify most of these parameters by editing the values in the input interfaces or model databases. After the input parameters are properly set and read, a simulation can be performed. The first step of the simulation is the initialization of numerous variables (e.g., soil temperature, moisture, Eh, and pH, soil C, N, and P pools, crop characteristics, production and consumption C and N gases, and fluxes of water, C, and N) in the model. This initialization sets all simulation variables to the starting condition.

Following read input data and model initialization, the model performs a simulation on a daily step for most of the processes each year. The model reads daily weather data provided by users and simulates the sub-models and processes under those weather conditions. After finishing one year simulation, the weather data of the next year is read, and the simulation of the next year is conducted. This continues until the requested number of simulated years is completed.

Each year, the simulation begins with parameterizing farming management practices (planting and harvest, crop residue return, tillage, irrigation, fertilization, manure amendment etc.) that coverts information of farming management practices into variables or factors influencing the soil environmental factors and/or simulated processes. For example, the model calculates changes of soil C and N pools based on the information of manure amendments (e.g., amounts of manure C and N inputs, N forms) and soil N pools based on the information of N fertilization (e.g., N rate, method of application, and type of fertilizers).

The soil climate sub-model simulates soil temperature and moisture profiles and water table dynamics by simulating soil physical processes (see the “Soil temperature”, “Soil moisture”, and “Soil Eh” sections). The model considers impacts of weather, soil properties, crop, and farming management practices on these soil environmental variables and simulates dynamics of soil environmental variables that regulate crop growth and all simulated biogeochemical processes.

Following the simulation of soil climate, growth and harvest of crops are simulated on a daily time-step over the full year. The model can simulate different types of crops based on the parameters of crop characteristics (see the “Modeling Crop Growth” section). The crop growth sub-model predicts daily growth and nutrition dynamics of crops and updates soil water and nutrients status based on the crop uptakes of soil water and nutrients.

The next simulated processes are nitrification and denitrification. In DNDCv.CAN, the nitrification and denitrification processes are simulated at an hourly step and are fully integrated as these two processes are tightly coupled in soils. In each hour of a given day, the model first calculates aerobic and anaerobic fractions of a soil layer (see the section “Modeling Redox Potential Dynamic and Soil Biogeochemistry under Aerobic and Anaerobic Conditions”) and then allocates the substrates (i.e., DOC, NH4+, NO3-, NO2-, NO, N2O) for the nitrification and denitrification processes into the aerobic or anaerobic fraction of the soil layer. Following these calculations, the model simulates the denitrification and nitrification processes by assuming that the denitrification happens solely under anaerobic conditions while nitrification happens solely under aerobic conditions (see the “Nitrification” and “Denitrification” sections). The model then summarizes production and consumption of N gases and calculates fluxes of N gases.

The next simulated sub-model is decomposition. Like nitrification and denitrification, there are several processes in the “decomposition” sub-model. The major processes include decomposition of each SOC sub-pool (see the “Decomposition” section), urea hydrolysis (see the “Urea hydrolysis” section), and NH3 volatilization (see the “Ammonia volatilization” section). These processes calculate daily DOC production rate, CO2 fluxes from soil heterotrophic respiration, soil organic C sequestration rate, urea hydrolysis rate, and NH3 fluxes.

After the simulation of the “decomposition” sub-model, the model determines if calculating fermentation and methanogenesis processes based on water table conditions. For upland cropping systems with deep water table, the model calculates soil CH4 uptakes. For non-upland systems (e.g., rice paddies, wetland), the model simulates CH4 production, oxidation, and transportation (see the “Methane dynamics” section).

At the end of a daily simulation, the model summarizes and outputs daily results of all the simulated variables (soil temperature and moisture, soil pH and Eh, soil C and N pools, crop biomass, water fluxes, and fluxes of C and N gases etc.). Following the simulation of the last day each year, the simulation proceeds to the next year and the process is repeated. This annual loop continues until the requested number of simulated years is complete. After the simulation is complete, all the variables are summarized and organized into annual results and written to output files.



**Figure 3 Overview of operations of DNDCv.CAN**

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

Following rainfall events, irrigation, or flooding, soil could shift from unsaturated to saturated conditions, causing soil oxygen (O2) depletion, and resulting in more oxidants involved in the reductive reactions. These reductive reactions usually include denitrification of nitrate, reductions of manganese (Mn4+), iron (Fe3+) and sulfate (SO42-), 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).

Eh = E0 + RT/nF \* ln([oxidant]/[reductant]) [Eq. 1]

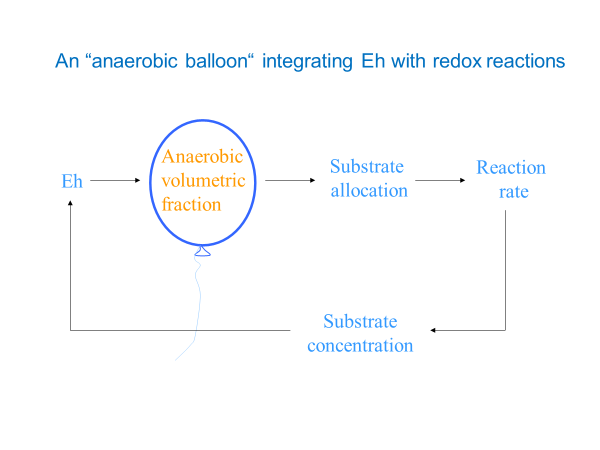
where Eh is redox potential of an oxidation-reduction system (V), E0 is standard electromotive force (V), R is the gas constant (8.314 J/mol/k), T is absolute temperature (273 + t, ºC), n is transferred electron number, F is the Faraday constant (96,485 C/mol), [oxidant] is concentration (mol/l) of dominant 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 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[oxidant] = a [DOC / (b + DOC)] \* [oxidant / (c + oxidant)] [Eq. 2]

where F[oxidant] is the oxidant reduced during a simulation 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 the model 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 (i.e., within the anaerobic volumetric fraction) and relatively aerobic micro-sites (i.e., outside of the anaerobic volumetric fraction). Based on these proportions, DNDC allocates the substrates (e.g., DOC, NH4+, NO3-, NO2-, NO, N2O, CO2 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 type 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, the model quantifies this effect as an “anaerobic balloon”, which swells or shrinks driven by the reduction/oxidation reactions (Figure 4). When 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., NO3-) will become the dominant oxidant in the soil. A new anaerobic balloon will be born, and swell driven by the NO3- depletion. More NO3- will be allocated within the anaerobic fraction during the ballon swelling. By tracking the formation and deflation of a series of anaerobic balloons driven by depletion of oxygen, NO3-, Mn4+, Fe3+, SO42-, and CO2, the model estimates soil Eh dynamics as well as production and consumption of the products from the reductive/oxidative reactions, including CO2, N2O and CH4 (Figure 4). With the anaerobic balloon concept, soil Eh dynamics are linked with substrate concentrations and C and N gases emissions from soils (Li et al., 2004).



**Figure 4 The “Anaerobic Balloon” concept for tracking processes under aerobic and anaerobic conditions simultaneously.**

DNDC's ability to simultaneously model nitrification and denitrification (Figure 5) by tracking anaerobic volume fraction is a key feature that allows the model to simulate N2O fluxes across a broad range of soil environmental conditions and microbial mediated pathways.



**Figure 5 DNDC tracks fraction of soil aerobic and anaerobic micro-sites and nitrification and denitrification processes, which dominate N2O and NO production and consumption.**

**6. Major Processes for Simulating C and N Gases Fluxes**

In this section, we discuss model processes that simulate C and N cycling, production and consumption of GHGs, and ammonia volatilization. Processes of decomposition, urea hydrolysis, NH3 production and volatilization, and NH3 absorption by plants are described in Table 1 and key equations involving N2O 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, NH3 production and emission, and NH3 absorption by plants.**

|  |
| --- |
| Process 1. Decomposition rate of organic carbon pool |
| dC/dt = CNR \* μ \* (S \* kl + (1-S) \* kr) \* [C] [Eq. 3]  Where [C] is organic C content (kg C ha-1), t is time (day), S is labile fraction of organic C compounds in the pool, (1-S) is resistant fraction of organic C compounds, kl is specific decomposition rate (SDR) of labile fraction (day-1), kr is SDR of the resistant fraction (day-1), 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 (day-1) 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-1), 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 NH4+, and [Urea] is concentration of urea (kg N ha-1). |
| Process 4a. NH4+/NH3 equilibrium under the condition without slurry manure application |
| NH4+ = NH3 + H+ [Eq. 6]  Ka = [NH4+][OH-] / [NH3(l)] [Eq. 7]  [H+] = 10-pH [Eq. 8]  H2O = H+ + OH- [Eq. 9]  Kw = [H+][OH-] [Eq. 10]  Ka = (1.416 + 0.01357 \* T) \* 10-5 [Eq. 11]  Kw = 10^(0.08946 + 0.03605 \* T) \* 10-15 [Eq. 12]  Where Ka is equilibrium constant, Kw is water dissociation constant, [NH4+], [OH-] and [NH3(l)] are NH4+, OH- and NH3(l) concentrations (mol l-1) in soil water, pH is soil pH, T is soil temperature. |
| Process 4b. NH4+/NH3 equilibrium with slurry manure application |
| NH4+ = NH3 + H+ [Eq. 13]  Ka = [NH4+][OH-] / [NH3(l)] [Eq. 14]  [H+] = 10-pH [Eq. 15]  H2O = H+ + OH- [Eq. 16]  Kw = [H+][OH-] [Eq. 17]  [Eq. 18]  [Eq. 19]  Where Ka is equilibrium constant, Kw is water dissociation constant, [NH4+], [OH-] and [NH3(l)] are NH4+, OH- and NH3(l) concentrations (mol l-1) in soil water, pH is soil pH, T is soil temperature. |
| Process 5a. NH3 diffusion from the bulk liquid to the interface of liquid phase |
| Fl = Kl \* ([NH3]bl – [NH3]il) [Eq. 20]  Where Fl is NH3 diffusion rate in liquid phase (kg N m-2 hr-1), Kl is NH3 mass transfer coefficient in the liquid boundary layer, [NH3]bl is NH3 concentration in the bulk liquid phase (kg N m-3), [NH3]il is NH3 concentration in the interface liquid phase (kg N m-3). |
| Process 5b. NH3 transfer from the interface of liquid phase to the bulk air |
| Fg = Kg \* ([NH3]ig – [NH3]ag) [Eq. 21]  Where Fg is NH3 transfer rate from the interface of liquid phase to the bulk air (kg N m-2 hr-1), Kg is NH3 mass transfer coefficient in the air boundary layer, [NH3]ig is NH3 concentration in the interface gas phase (kg N m-3), [NH3]ag is NH3 concentration in the air (kg N m-3). |
| Process 5c. Equilibrium between NH3 in the interface of liquid and NH3 in the interface of gas phase |
| [NH3]ig = Kh \* [NH3]il [Eq. 22]  Where [NH3]ig is NH3 concentration in the interface of gas phase (kg N m-3), [NH3]il is NH3 concentration in the interface of liquid phase (kg N m-3), Kh is Henry’s coefficient. |
| Process 6a. NH4+ adsorption by clay |
| FIXNH4 = (0.41 - 0.47 \* log([NH4])) \* (CLAY/CLAYmax) [Eq. 23]  Where FIXNH4 is proportion of adsorbed NH4+, [NH4] is NH4+ concentration in the soil liquid (g N kg-1), CLAY is clay fraction in soil, CLAYmax is maximum clay fraction (0.63). |
| Process 6b. NH3 absorption by plants in field |
| PlantUp\_NH3 = Vg \* Air\_NH3 \* LAI \* 0.864 [Eq. 24]  Vg = MaxVg \* F(plant-N) \* F(lsm) [Eq. 25]  F(plant-N) = Plant-N(act) / Plant-N(opt) [Eq. 26]  F(lsm) = LSM (act) / LSM(max) [Eq. 27]  Air\_NH3 = Base\_NH3 + Flux\_NH3 \* 10^9 / V(canopy) \*LAI / (LAI + k2) \* k3 [Eq. 28]  Where PlantUp\_NH3 is daily NH3 absorption by plant, Vg is NH3 deposition velocity (m s-1), MaxVg is maximum velocity (0.050 m s-1), Plant-N(act) is N content in crop (kg N ha-1), Plant-N(opt) is optimum N content (kg N ha-1) in crop, LSM(act) is water content on leaf surface (cm), LSM(max) is maximum water content on leaf surface (cm), Base\_NH3 is atmospheric background NH3 concentration (μg m-3), Flux\_NH3 is daily NH3 flux (kg N ha-1) from soil, V(canopy) is volume of the room from ground to the top of canopy (m3), LAI is leaf area index, and k2 and k3 are coefficients. |

**6.1. Decomposition**

Decomposition is a process describing degradation of 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 CO2 production, and another part of the SOC used for the microbial construction. During the decomposition, labile C will be gradually lost with resistant C becoming relatively more abundant in the soil. The model simulates SOC decomposition by simultaneously calculating the decomposition rate for each of the SOC sub-pools (including litter, microbes, humads (i.e., active humus), and passive humus). Figure 6 shows the sequential decomposition processes, 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 soil 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 SOC mineralization 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 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 6. SOC pools and decomposition processes.**

**6.2. 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(NH2)2). During the hydrolysis, a molecule of urea is converted to two molecules of ammonium with a hydroxyl (OH-) released (Eq. 29).

CO(NH2) 2 + 3H2O = 2NH4+ + HCO3− + OH- [Eq. 29]

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 the temperature is favorable. The hydroxyl released from the urea hydrolysis elevates the soil pH which in turn affects a series of biogeochemical processes including NH3 volatilization.

In DNDCv.CAN, the function of simulating urease activity has been further modified because the original function may overestimate hydrolysis rates under very dry conditions (Jiang et al., 2023). The urease activity calculation proposed by Ferguson and Kissel (1986) has been adopted to reduce urease activity as soil moisture approaching the permanent wilting point. In addition, the original fixed urease inhibitor efficiency has been changed into dynamic in DNDCv.CAN (Jiang et al., 2023). The degradation of N-(n-Butyl)thiophosphoric triamide (NBPT) inhibitors over time is calculated using the following equation based on Engel et al. (2015).

Y = -5.93 + 1.13X [Eq. 30]

where Y is the half-life of NBPT in days, and X is the impact of soil pH on the effectiveness of NBPT. The pH range (X) for this function is set to a minimum pH of 5.25 and maximum pH of 8.75.

**6.3. Ammonia volatilization**

When ammonium (NH4+) is applied through fertilization, manure amendment, or produced from either decomposition or urea hydrolysis, the NH4+ dissolved in the soil liquid will keep in equilibrium with the dissolved ammonia (NH3) (Eq. 31).

NH4+ = NH3↑+ H+ [Eq. 31]

The reaction can shift in either direction depending on the NH4+concentration, NH3 concentration, and pH in the liquid phase. To calculate the reaction rate, two dissociation constants for the NH4+/NH3 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 4a in Table 1) following Glasstone (1946) and Sutton et al. (1993). As soon as NH3 is formed, it can diffuse to the liquid/air interface driven by the NH3 concentration gradients. A two-film module has been adopted in DNDC to quantify the NH3 emissions from the soil surface. Following De Visscher et al. (2002), Henry’s law and NH3 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. Ammonium adsorption is modeled as logarithmic relationship between ammonium concentration and clay fraction in the soils.

Congreves et al. (2016) has integrated new equations into DNDCv.CAN to calculate NH3 volatilization from slurry applications. While the principle of simulating NH3 volatilization from slurry applications is generally identical between DNDCv.CAN and DNDC, the calculations of Ka and Kw are different (Eq. 18 and Eq. 19). In addition, DNDCv.CAN has linked the transport of total ammonium nitrogen (TAN) in slurry water down the soil profile with soil hydrology processes, and has calculated the pH of the soil and slurry solution and used the solution pH, instead of soil pH, to calculate dissociation of the NH4+/NH3 following the slurry applications (Congreves et al., 2016). DNDCv.CAN also provides input parameters to enable modifications of influences of windspeed and soil depth on NH3 volatilization. The reductions of NH3 volatilization with deeper soils represent the diffusivity ease of NH3 from depth along with the binding of NH3 to soil colloids within the soil matrix.

Ammonia can be absorbed by crops/vegetation. The model simulates ammonia adsorption on crops based on daily ammonia flux and biophysical conditions of the crop leaf area index (LAI), plant heights, and leaf moisture). Process 6a and b in Table 1 describe ammonium adsorption and ammonia adsorption by crops, respectively.

**6.4. Nitrification**

Under aerobic conditions, NH4+ can be oxidized to NO2- and further to NO3- by ammonium oxidizers (Eq. 32) (McGill et al., 1981; Van Veen and Frissel, 1979). This two-step process is called nitrification. During nitrification, a certain amount of NO or N2O can be evolved as a byproduct (Bremner and Blackmer, 1978; Parton et al., 1988).

NH4+ + O2→ NO2− + 4H+ + 2e−

NO2− + H2O → NO3− + 2H+ + 2e- [Eq. 32]

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 NH4+. In DNDC, the growth and death rates of nitrifiers are set as functions of DOC and soil moisture (Equations 33 to 34 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 NH4+ availability and pH (Eq. 36 in Table 2). DNDCv.CAN also enables the modifications of the growth rate of nitrifiers and rate of nitrification through changing relevant parameters in input interfaces. Based on Bremner and Blackmer (1981), the nitrification derived N2O is a fraction of the nitrification rate (Eq. 39 in Table 2).

**Table 2. Key equations for simulating nitrification.**

|  |  |
| --- | --- |
| Relative growth (dG/dt) and death rates (dD/dt) of nitrifiers |  |
|  | [Eq. 33] |
|  | [Eq. 34] |
| Where [DOC] is dissolved organic carbon content (kg C ha-1), Fm is a soil moisture factor, and Nitrifier is biomass of nitrifier. | |
| Net increase in nitrifier biomass |  |
|  | [Eq. 35] |
| Nitrification rate |  |
|  | [Eq. 36] |
| Where [NH4+] is concentration of ammonium (kg N ha-1) and pH is the soil pH. | |
| Soil moisture factor in nitrification |  |
|  | [Eq. 37] |
| Where WFPS is the soil water content in water filled porosity. | |
| Soil temperature factor in nitrification |  |
|  | [Eq. 38] |
| Where T is the soil temperature. | |
| N2O production through nitrification |  |
|  | [Eq. 39] |
| Where RN is the nitrification rate as in Eq. 28. |  |

**6.5. Denitrification**

Denitrification is a series of microbe-mediated reactions that sequentially reduce NO3- to NO2-, NO, N2O, and finally dinitrogen (N2) (Eq. 40). As reductive reactions, the denitrifying sequence can occur only under anaerobic conditions.

NO3− + 2e− → NO2− + e− → NO + e−→ N2O + 2e− → N2 [Eq. 40]

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., NO3-, NO2-, NO, or N2O), 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 model framework (see the section “Modeling Redox Potential Dynamic and Soil Biogeochemistry under Aerobic and Anaerobic Conditions”). All denitrifiers are capable of anaerobic growth only in the presence of DOC and nitrogenous oxides (i.e., NO3-, NO2-, NO, or N2O). 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 41 to 43 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 41 and 42 in Table 3). The denitrifier death rate is modeled as proportional to denitrifier biomass (Eq. 44 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 DNDCv.CAN provides an additional parameter that enables the modification of the growth rates of denitrifiers.

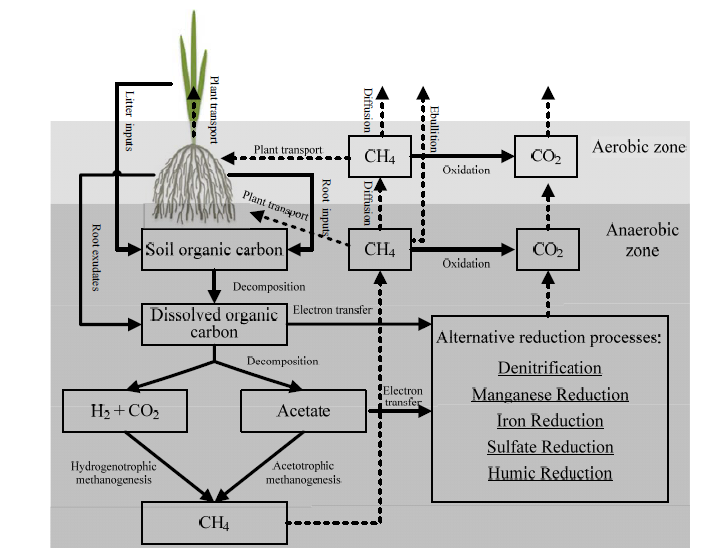
The effects of soil pH or temperature on denitrification are modeled in DNDC based on observations reported by a number of studies (Mueller et al., 1980; Klemedtsoon et al., 1978; Burford and Bremner, 1975; Stanford et al., 1975a; Khan and Moore, 1968; Wijler and Delwiche, 1954; Focht, 1974; Leffelaar 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 49 and 50 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. 45 in Table 3). CO2 production is calculated as the difference between the total amount of consumed C and the amount used for cell synthesis (Eq. 46 in Table 3). Consumptions of NO3-, NO2-, and N2O are calculated with Pirt's equation (Eq. 47 in Table 3). 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 (NO3-denitrifier + NO2-denitrifier + N2O denitrifier) (Eq. 47 in Table 3). The DNDCv.CAN model also provides a parameter to modify the N2O consumption rate. Based on the growth rates of denitrifiers and the C/N ratio in the bacteria, the assimilation of N during denitrification is calculated (Eq. 48 in Table 3). A C/N ratio (by weight) of 3.45 is used based on the chemical composition of denitrifiers (C6H10.8N1.5O2.9), in accordance with data reported for *Paracoccus denitrificans* (Verseveld and Stouthamer, 1978).

**Table 3. Key equations for simulating denitrification.**

|  |  |
| --- | --- |
| Relative growth rates of NOX denitrifiers |  |
|  | [Eq. 41] |
|  | [Eq. 42] |
|  | [Eq. 43] |
| Where uNOx,max is the maximum growth rate of NO3-, NO2-, NO, or N2O denitrifiers, DOC is dissolved organic carbon content (kg C ha-1), NOx is concentration of NO3-, NO2-, NO, or N2O in soil water (kg N ha-1), KC is half-saturation value of soluble C in the Monod model (kg C m-3 soil water), KN is half-saturation value of NO3-, NO2-, NO, or N2O in the Monod model (kg N m-3 soil water), FT is a temperature factor, FPH-NO3, FPH-NO2, FPH-NO, and FPH-N2O is soil pH factors, and Denitrifier is biomass of denitrifier. | |
| Relative death rates of denitrifiers |  |
|  | [Eq. 44] |
| Where MC is maintenance coefficient of C (kg C kg-1 C hr-1) and YC is maximum growth yield on soluble carbon (kg C kg-1 C). | |
| Consumption of DOC and CO2 production through denitrification |  |
|  | [Eq. 45] |
|  | [Eq. 46] |
| Consumption of NOX through denitrification |  |
|  | [Eq. 47] |
| Where YNO3, YNO2, YNO, and YN2O is the maximum growth yield on NO3-, NO2-, NO, or N2O (kg C kg-1 N), MNO3, MNO2,MNO,and MN2O is the maintenance coefficient of NO3-, NO2-, NO, or N2O (kg N/kg/hr), and N is the total nitrogen as the sum of NO3-, NO2-, NO, and N2O (kg N ha-1). | |
| Assimilation of N during denitrification |  |
|  | [Eq. 48] |
| Where C/N denitrifier is C/N ratio in denitrifiers. |  |
| Soil temperature factor in denitrification |  |
|  | [Eq. 49] |
| Where T is the soil temperature. |  |
| pH factor in denitrification |  |
|  | [Eq. 50] |
| Where pH is the soil pH. | |

**6.6. Methane dynamics**

The rate of methane emission is predicted by modeling its production, consumption, and transport processes (Figure 7). 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., H2 and DOC) and acceptors (i.e., NO3-, Mn4+, Fe3+, SO42-, and CO2). The simulation of SOC decomposition has been described in 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., NO3-, Mn4+, Fe3+, SO42-, and CO2) may become involved in reductive reactions. Soil Eh gradually decreases along with the consumption of these oxidants, and DNDC simulates denitrification, reductions of Mn4+, Fe3+, and SO42-, 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 NO3-, Mn4+, Fe3+, and SO42-, when soil Eh is below -150 mV (Li et al., 2004). Methane consumption is simulated as an oxidation reaction involving electron exchange between CH4 and oxygen. In the model, CH4 production and oxidation can occur simultaneously within a soil layer (around 2 cm thick) but within relatively aerobic and anaerobic sub-layers, whose volumetric fractions are determined by Eh calculations (Li, 2007). Redox potential, soil temperature, pH, and the concentrations of electron donors and acceptors are the major factors controlling the rates of CH4 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).

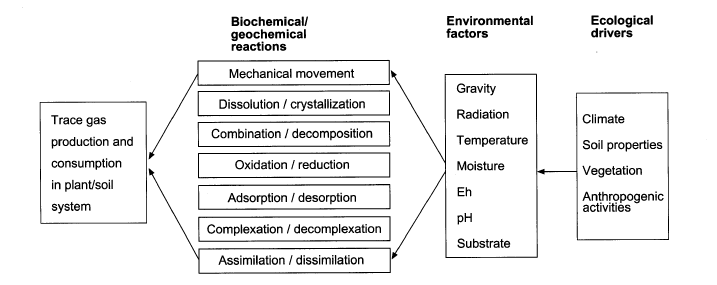


**Figure 7 The framework for simulating soil biogeochemistry and methane dynamics in the modified DNDC.**

**7. Modeling Environmental Factors**

All biogeochemical reactions are controlled by a group of environmental factors such as soil temperature, soil 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 8). 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, fertilization, manure application, tillage etc.). Like the DNDC model, daily weather data (e.g., air temperature, precipitation, solar radiation, and wind speed), soil properties (e.g., bulk density, texture, SOC content, and pH), vegetation characteristics, and field management activities are used in DNDCv.CAN as inputs to determine the dynamics of temperature, moisture, pH, Eh, and substrate concentration in soil profile.

Farming management practices, 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. Organic C and N bound in the manure are released through decomposition and distributed into the relevant soil C and N pools and 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.



**Figure 8 The framework of linking soil environmental factors with biogeochemical reactions to simulate production and consumption of trace gases in agricultural soils.**

**7.1. Soil temperature**

Temperature is one of the most important factors affecting biochemical or geochemical reactions. Simulations of soil temperature vary across different depths. The DNDC 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.

DNDCv.CAN has incorporated functions to simulate influences of snow depth, canopy cover, and crop residue on soil temperature (Dutta et al., 2018). The influence of snow depth on soil temperature is calculated using Equation 51 based on Rankinen et al. (2004).

[Eq. 51]

where, T\* is the soil temperature under soil snow depth, T is the soil temperature, fS (m−1) is an empirical snow parameter from Rankinen et al. (2004), and DS is snow depth (m).

The influences of canopy cover and crop residue on soil temperature are calculated using the following equation (Sándor & Fodor, 2012):

[Eq. 52]

where, T\*\* is the soil temperature under the influence of canopy cover and the presence of residue, T is the soil temperature, LC is the fraction of radiation transmitted through a canopy, and RF is the crop residue factor.

The fraction of radiation transmitted through a canopy is estimated according to the Beer–Lambert law using the following equation:

[Eq. 53]

where k is the extinction coefficient, LAI (m2 m-2) is the leaf area index, and α is the average canopy albedo.

**7.2. 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. The DNDC model simulates soil moisture in each layer by calculating both surface and vertical water movements (Figure 9), 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, precipitation, solar radiation, humidity, and wind speed), soil properties (e.g., texture, field capacity, wilt point, hydrological conductivity, and previous soil water availability), crop growth, and FMPs (irrigation, flooding, film mulch etc.).

A diagram of a soil layer

Description automatically generated with medium confidence

Figure 9 **Schematic of DNDCv.CAN for simulating hydrological processes.** Hydrological processes in both DNDC and DNDCv.CAN are illustrated. Shaded areas show different algorithms between DNDCv.CAN and DNDC. The figure was from Smith et al., (2020).

DNDC's soil hydrological processes were enhanced in DNDCv.CAN (Figure 9) (Smith et al., 2020). Specifically, the following changes were made.

1. The model interface was restructured to allow for a heterogeneous and deeper soil profile. Soil properties can be defined by depth. Model users can specify the depth of the soil profile up to 200 cm (the default depth is 50 cm in the original DNDC model) and define properties for up to ten user defined depths. The simulation depth was also adjusted from 50 cm to 200 cm (Figure 9). The model can not only simulate soil hydrology but also all biogeochemical processes up to a 200 cm depth.

2. Root penetration and density functions have been incorporated into the model. The root penetration and density functions affect crop water uptake and therefore affect soil moisture dynamics. The DNDC model calculates a linear estimate of root penetration to a maximum depth of 50 cm, without considering root density. In DNDCv.CAN, a root penetration equation based on growing degree days (GDD) was incorporated. The equation, expressed in terms of PGI (Plant Growth Index), is as follows.

[Eq. 54]

where RootZ is the depth of root penetration, PGI is the fraction of accumulated degree days required for a plant to reach maturity, RootZMin is the planting depth, PGILag accounts for the period between planting and start of root penetration, kRZ is the root depth penetration rate, RootZMax is the maximum root penetration depth (a model input parameter).

An algorithm for root distribution that extends the rooting depth of fine roots by an additional 30% was also employed in DNDCv.CAN. The root density declines logarithmically to the root penetration depth (RootZ) followed by a linear decrease to zero at 1.3RootZ. The relative root length distribution is as follows.

[Eq. 55]

where a is the shape parameter (default value: 2.0) describing root distribution with increasing soil depth.

3. The cascade flow approach for simulating vertical water flow movement has been improved by limiting the movement above field capacity based on soil water status. The unsaturated conductivity is calculated using the following equation:

[Eq. 56]

where K is hydraulic conductivity, KSAT is saturated hydraulic conductivity, θ is actual, θr residual, and θs saturated soil water content (cm3 cm−3), n is a constant with the default value of 3.5.

4. The DNDCv.CAN model has incorporated a function to simulate fluctuating water tables. A water table slowly builds up from the bottom soil layer with deep seepage at the lower boundary. The water table is calculated based on the mass balance of incoming water from precipitation and irrigation and outgoing water from runoff, evapotranspiration, tile drainage, deep seepage, and change in soil water content in unsaturated layers. For the purposes of estimating tile flow rate, the water table height was calculated at the top of the saturated soil layer closest to the soil surface.

5. A tile drainage sub-model was incorporated into the DNDCv.CAN model. The drainage discharge rate is calculated using the Hooghoudt equation (Skaggs et al., 2012):

[Eq. 57]

where q (cm h−1) is the drainage discharge rate, Ke (cm h−1) is the effective lateral hydraulic conductivity, m is the water table level above the drain at midpoint between the drains, de is the equivalent depth to the impermeable (or restrictive) layer below the drain, and L is the drain spacing.

**7.3. Soil Eh**

The processes of decomposition, nitrification, denitrification, and methanogenesis producing GHGs (CO2, N2O, and CH4) are typical reductive-oxidative reactions, which occur through electron exchange between the substrates. The environmental Eh determines the occurrence of the reactions (Stumm and Morgan, 1981). Under aerobic conditions, the Eh values in soils vary between 100 and 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 heavy rainfall, oxygen in the soil will be depleted and lead to anaerobic conditions (Eh -300 to 0 mV), under which reductive reactions such as denitrification or methanogenesis will occur. In reality, the aerobic and anaerobic micro-sites can simultaneously exit in the same soil layer although their volumetric proportions could vary according to the bulk Eh of the soil. The approach for modeling Eh is provided in the section of "Modeling Redox Potential Dynamic and Soil Biogeochemistry under Aerobic and Anaerobic Conditions".

**7.4. Soil pH**

Environmental acidity represented as pH determines the 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 values. This increase in soil pH will lead to increases of NH3 volatilization by shifting the NH4+/NH3 equilibrium. Soil pH also influences consumptions of NO3-, NO2-, and N2O in denitrification. DNDCv.CAN tracks the variation of soil pH by counting H+ production or consumption in the biogeochemical reactions at a daily time step. Relevant processes (e.g., urease activity, hydrolysis, NH4+/NH3 equilibrium, NH3 dynamics, and NH4+ adsorption) are discussed above.

**7.5. Substrate concentration**

The rates of biogeochemical reactions related to CO2, CH4, N2O, NO, or NH3 production and/or consumption are not only regulated by the environmental 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. DOC concentration in the soil is calculated 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 methanotrophs) or water movements (runoff and leaching) (Deng et al., 2021). 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, the model calculates NH4+ and NO3- concentrations of each soil layer at a daily time step. Soil NH4+ content increases due to external inputs, decomposition, and ammonification, and decreases due to nitrification, NH3 volatilization, adsorption, plant uptake, and runoff. Soil NO3- content increases due to external inputs, nitrification, and decreases due to denitrification, plant uptake, and water-induced losses (runoff and leaching). The modeled concentrations of DOC, NH4+ and NO3- are utilized to calculate the rates of the relevant biogeochemical processes as described above.

**8. Modeling Crop Growth**

In DNDC, crop biomass dynamics are simulated at daily time step by considering the effects of several environmental factors on plant growth, including solar radiation, air temperature, and availability of soil water and N (Figure 10). 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 10 illustrates, daily crop growth and yields are controlled by complex interactions of weather, soil conditions and crop physiological characteristics. Note that the modifications in DNDCv.CAN for simulating soil moisture (please refer to the section “Soil moisture”) could influence the simulation of crop growth through changing water and N dynamics of different soil layers and water and N uptakes. 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 10 DNDC models interactions of weather, soil conditions and crop physiological characteristics for predicting daily crop growth and yields.**

The DNDCv.CAN model has been further developed to better simulate alfalfa production with winterkill effects (He et al., 2019). The processes of cold hardening and dehardening based on the ALFACOLD model (Kanneganti et al., 1998a, b) have been integrated into DNDCv.CAN to predict winterkill impacts on alfalfa growth. In DNDCv.CAN, daily rate of increase in cold hardening (HRI, °C d−1) was computed as follows:

[Eq. 58]

where ETHRI (dimensionless, -1 to 1) represents the effect of average daily crown temperature (CRTMP, °C) on the potential rate of hardening (CHRMX, °C d−1). The ETHRI is a function of soil temperature at 3 cm depth.

The daily rate of dehardening (DRI, °C d−1), which results in a decrease in cold tolerance, is calculated as follows:

[Eq. 59]

where ETDRI (dimensionless, 0 to 1) represents the effect of average daily crown temperature on the potential rate of dehardening (CDRMX,°C d−1). The ETDRI values are based on the previous experiments (Paquin and Pelletier, 1980; McKenzie et al., 1988; Kanneganti et al., 1998a).

The state of cold tolerance is quantified by CTT (°C), which is equivalent to the subzero temperature that a crop can tolerate without being killed. It is calculated as follows:

[Eq. 60]

The difference between HRI and DRI represents the daily rate of net increase or decrease in cold tolerance. The CTT (°C) and CTMX (maximum temperature of cold tolerance, °C) are negative values, indicating subzero temperatures. CTT is initialized to 0 °C at the start of a simulation.

Plant death caused by winterkill is quantified by a plant death factor (PDF, d-l), which represents a fraction of plant population (plants m−2) dead in a day, as follows:

[Eq. 61]

where CRTMP is the average daily crown temperature which is estimated using soil temperature at 3 cm depth and PDFMX (d–l °C−1 below CTT) represents cultivar specific potential rate of plant death with a default value of 0.12 d–l °C−1.

The calculation and incidence of a PDF event is applied as a cumulative scalar (PDFcummulative) that acts to reduce the potential crop N demand/C biomass growth in alfalfa to represent the reduction in plant population due to winterkill over time (e.g., 0.0 = no winterkill effect and 1.0 representing 100% loss in plant population).

The winterkill effect (WE, %) on alfalfa yield for each overwinter period was modelled based on potential yield reduction of the subsequent year. The cumulative winterkill effect (CWE, %) is calculated based on the initial potential yield and total yield reduction due to winterkill as follows.

[Eq. 61]

[Eq. 62]

where SPYR (kg ha−1) is potential yield reduction of subsequent year, SPY (kg ha−1) is the potential alfalfa yield of subsequent year, TPYR (kg ha−1) represents the total potential yield reduction for all growing years because of plant stand loss and IPY (kg ha−1) is the initial potential yield of alfalfa.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
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