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Advance in a terrestrial biogeochemical model—DNDC model

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ABSTRACT

Global climate change is one of the most important issues of contemporary environmental safety. Quantifying regional or global greenhouse gas (GHG) emissions and searching for appropriate mitigation measures have become a relatively hot issue in international global climate change studies. The high temporal and spatial variability of GHG emissions from soils makes their field measurement at regional or national scales impractical. To develop emission factors for a wide range of management practices such as those given in the Intergovernmental Panel on Climate Change Tier I methodology are often considered as a convenient technique to estimate emissions, but these can result in substantial errors when applied to specific geographical regions. Accordingly, considering the complexity of greenhouse gas production in soils, process-based models are required to quantify and predict the GHG emissions, and also interpret the intricate relationships among the gas emissions, the environmental factors and the ecological drivers. Several detailed biogeochemical process-based models of GHG emissions have been developed and accepted in recent years to provide regional scale estimate of GHG emissions and assess the mitigation measures. Among these the DNDC (Denitrification–Decomposition) model, as a process-based biogeochemical model, is capable of predicting the soil fluxes of all three terrestrial greenhouse gases: nitrous oxide (N_2O), carbon dioxide (CO_2), and methane (CH_4), as well as other important environmental and economic indicators such as crop production, ammonia (NH_3) volatilisation and nitrate NO_3^- leaching. Originally developed as a tool to simulate GHG emissions generated from agro-ecosystem, DNDC has since been expanded to include ecosystems such as rice paddies, grazed pastures, forests, and wetlands, and the model has attracted worldwide attention to simulate carbon and nitrogen biogeochemical cycles occurring in global ecosystems. This paper introduces the scientific basis underlying the modeling of greenhouse gas emissions from terrestrial soils, brings together the worldwide research undertaken on a wide range of ecosystems to test and verify, improve and modify, and apply the DNDC model to estimate GHG emissions from these systems, and furtherly sums up the advantages and disadvantages of the model for providing a reference for the application and development of the model. Most studies showed that there was a good agreement between the simulated and observed values of CO_2, CH_4 and N_2O emissions from arable, forest and grassland fields at different geographical locations over the world. However, some discrepancies still existed between observed and simulated seasonal patterns of CH_4 and N_2O emissions. Moreover, the DNDC model was mainly tested against experimental data on GHG emissions, but there were a few validations on NO_3^- leaching, soil water dynamics, NH_3 volatilisation which could greatly impact the GHG emissions. With the high development of society and economy, China had been facing a huge challenge between food production and environmental protection. Therefore, it was an urgent task to search optimal measures for optimizing land resource use, increasing crop productivity and reducing adverse environmental impacts. Process-based biogeochemical modeling, as with DNDC, can help in identifying optimal strategies to meet the needs. In future, the DNDC model need to not only improve the capability of predicting the GHG emissions, but also the accuracy of simulating the NO_3^- leaching and soil water dynamics for quantifying the non-point source pollution through modifying the parameters of the model or combining with other models, as SWAT model. The DNDC model will play more and more important role in future studies on global change.

1. Introduction

In recent years, extreme events induced by global climate change such as tsunamis, hurricanes, heavy rain and drought, have been threatening hundreds of millions of people's lives. The

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international community is working hard to strengthen the control of global climate change. Therefore, as the main greenhouse gases, carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O), have been attracting scientists and government great attentions. Agricultural soils are the main source of the three gases. A study indicated that soil organic matter decomposed by microorganisms can release into the atmosphere in the form of CO_2, the paddy soils in the long-term flooding condition can produce CH_4 by fermentation, N_2O was produced primarily through nitrification and denitrification processes [1]. The fourth assessment report of IPCC pointed out that agriculture accounted for an estimated emission of 5.1–6.1 G t CO_2-eq/yr in 2005 (10–12% of total global anthropogenic emissions of greenhouse gases (GHGs)). CH_4 contributed 3.3 G t CO_2-eq/yr and N_2O 2.8 G t CO_2-eq/yr. Of global anthropogenic emissions in 2005, agriculture accounted for about 60% of N_2O and about 50% of CH_4 [2]. Therefore, understanding the impacts of human activities on greenhouse gas emissions from productive soils is vital for mitigating negative effects on climate change while continuing to feed the world increasing population. Quantifying agricultural GHGs emissions not only plays an important role in seeking suitable mitigation measures, but also can provide basis for rationally assessing national responsibility and obligation of GHGs mitigation, and hence become an essential task in current scientific research. Many countries use the IPCC default methodology (the 'emission factor') for calculating GHGs emissions from agricultural soils for their national inventories [3]. The emission factor is deduced from a limited number of observations but represents an average value over all soil types, climate conditions and management practices. Therefore, there is a high degree of uncertainty associated with the emission factor method to evaluate regional or national GHGs emissions. In addition, direct measurement of greenhouse gas emissions through field observation is a normal method. However, the method used for inventory purposes is impractical as it would require many measurements to be made over large areas and for long periods of time. For these reasons the development of a more process-based approach is desirable. In fact, models offer the possibility to simulate the intricate processes in the soil and the change of GHG emissions. Process-based models, such as CENTURY, TEM, ROTHC and DNDC model, were widely accepted and used to predict the impact of various agricultural management practices on net GHG emissions by analyzing the interactions between management practices, primary drivers (climate, soil type, crop type, etc.), and biogeochemical reactions. In comparison with several existing models capable of simulating GHG emissions, DNDC has an advantage because it cannot only simultaneously predict CO_2, CH_4 and N_2O emissions from agricultural, grassland, and forest ecosystems, but also assess overall impacts of various management practices on crop yield and nitrate leaching. It has been used and expanded by many research groups covering a range of countries and crop systems. This paper provides a review of the scientific basis and the latest research progress of the DNDC model, summarizes its advantages and defects, and reports how it has been validated and used. We hope that these efforts in this paper can enhance further applicability of the DNDC model.

2. The DNDC model

The Denitrification–Decomposition or DNDC model was originally developed from New Hampshire University of USA for predicting carbon sequestration and trace gas emissions from upland agricultural lands [4,5]. The core of DNDC was built up by integrating a group of biochemical and geochemical reactions commonly occurring in agroecosystems, which governed carbon (C) and nitrogen (N) transport and transformation in the plant–soil–climate systems, including CO_2, N_2O and CH_4 emissions, soil organic carbon (SOC) dynamics, and so on. DNDC is recognized as one of the most successful biogeochemical model which is suitable for a wide range of agroecosystems across any climatic zone [6–8]. The DNDC model consists of six sub-models for simulating soil climate, plant growth, decomposition, nitrification, denitrification and fermentation, respectively. The soil climate sub-model calculates soil temperature and moisture profiles based on soil physical properties, daily weather and plant water use. The plant growth sub-model tracks crop growth and partitioning of the biomass into grain, stalk and roots according to crop types, air temperature, soil moisture, management practices (i.e., fertilizer application, irrigation, tillage, harvest, grazing, etc.). The decomposition sub-model simulates production and decomposition of soil organic matter driven by the soil microbial respiration. The nitrification sub-model calculates growth of nitrifiers and oxidation of ammonium to nitrate. The denitrification sub-model operates at an hourly time step to simulate denitrification and the production of nitric oxide, nitrous oxide, and dinitrogen. The fermentation sub-model simulates methane production and oxidation under anaerobic conditions. The six sub-models interact to enable DNDC to simulate a relatively complete suite of biochemical and geochemical processes occurring under both aerobic and anaerobic conditions. More information about the concepts or mathematics of the model can be found in former publications [7,9–11]. The DNDC model is available via the internet (http://www.dndc.sr.unh.edu).

3. DNDC model validation

The validation is indispensable for model further application. During the past two decades, the DNDC model has been independently tested and applied for soil C and N studies in 20 countries including China with promising results. The validation is to compare the goodness of fit between the field observations and the model simulations driven by practical parameters. The parameters supporting for the model running include daily climatic data (i.e., temperature and rainfall), soil property (i.e., soil density, texture, initial SOC and pH), land use (i.e., crop type and rotation system), and management practices (i.e., tillage, fertilizer, irrigation, crop residue returned rates and grass cutting). The outputs of the model include crop yield, GHG emission rates such as N_2O, CH_4, CO_2, and so on.

Although each simulating process embedded in DNDC is well-founded, it still needs to test whether the model can interpret and extrapolate the field observations in different climate, soil and management conditions, and the more validations the better. DNDC was widely tested by researchers in many countries when the model was first published [4,5]. Subsequently, six long-term field data across the world were collected by Li et al. [9] and conducted to test the model's performance of simulating SOC dynamics. The simulation results were all consistent with the measurements. In 1995, nine models including DNDC were tested with 12 long-term SOC dynamics field datasets from different sites over the world, of which the DNDC was considered as one of the four better models [8]. Recently, DNDC was intensively validated for predicting N_2O, CH_4, CO_2 emissions (Table 1). Most of the test results indicated that the model was capable of simulating the magnitudes and dynamics of C and N pools with limited modifications, which implied that DNDC had contained leading factors and courses of terrestrial biogeochemical processes. However, since the greenhouse gas emissions from agricultural soils are very sensitive to climate, soil types, crop systems, etc., the discrepancies between simulations and observations of GHG emissions still existed across different environment conditions. For example, Babu et al. [12] used N_2O and CH_4 emission fluxes observed from 10 different rice paddy experimental sites in Indian for the validation of

Table 1
The worldwide validation of the DNDC model.

Crop system	Validation	Nation and region	Data source
Winter wheat, summer maize, rice	NO, N_2O, CH_4, NH_3	China, Costarica, USA	[10]
Corn/rape, soybean/winter wheat	N_2O	China	[15,16]
Rice	N_2O, CH_4	China	[17,18]
Winter wheat/summer maize	CO_2	China	[19]
Cotton, winter wheat/summer maize	CO_2	China	[20]
Soybean	N_2O	China	[21]
Barley, grassland	N_2O	Ireland	[22]
Rice/winter wheat	Crop yield, CH_4, N_2O	Indian	[23]
Soybean/corn	NO_3^- leaching	USA	[24]
Grassland	N_2O	Belgium	[25]
Cropland	N_2O	Belgium	[26]
Grassland	N_2O, soil moisture	USA, Scotland, Germany	[27]
Cropland	CO_2, N_2O, CH_4	Canada	[28]
Grassland	N_2O	Ireland	[29]
Rice	Yield, CH_4, N_2O	Indian	[30]
Cropland	N_2O	Canada	[31]
Cropland	N_2O, soil water	Canada	[32]
Grassland	N_2O, CO_2	Australia	[33]
Grassland	N_2O, soil moisture	China	[34]
Rice	CO_2, N_2O, CH_4	China	[35]

the DNDC. The results showed that the differences between simulations and measurements existed but were all less than 20%. It needed to further modify internal coefficients embedded in DNDC to improve the simulation accuracy of CH_4 emissions from rice paddy. Beheydta et al. [13] selected N_2O emissions from 22 long-term sites in Belgium to test the model, the results showed that the model had good performances in simulating N_2O emissions from agricultural soils but grassland soils. Tamon et al. [14] also found that DNDC with a few modifications can predict CH_4 emissions better from rice paddy soils in Japan. A report by Xie and Li [21] showed that the model can simulate the dynamics of N_2O emissions during soybean growth period in Beijing, but the model underestimated N_2O emission fluxes during the drought and non-agricultural activity periods. Therefore, it still needed to continue testing the model against more observations across climate zones, soil types and management regimes for the validations and modifications of the DNDC.

4. Regional application of the model

If a biogeochemistry model was only to be of use at site scale, it might only play a limited role because almost all the serious eco-environment issues happened in a large scale, and were managed or governed in regional scale. And thus only the scientific results that obtained from the large scale or national scale can effectively promote establishing new policy or legislation. DNDC had the function of regional modeling which was extended from site modeling. For the regional modeling, we usually need to partition the whole research region into many grid cells, and assume all of the attributes in each grid cell are uniform. Only on the basis of the presetting, we can run the model grid cell by grid cell across the entire region to obtain regional results. The input parameters of each grid cell for model running (e.g., climate, soil, crop type, management practices, etc.) were advance compiled to geographic information system (GIS) databases to support modeling calculations at regional scale. The DNDC will run twice with the maximum and minimum of the most sensitive factor (e.g., SOC) for each grid to produce two values. The two values will form a range, which is assumed to be wide enough to cover the "real" value with a high probability, although quantification of the uncertainty still remains as a challenge. The region modeling result equals the sum of each grid's result. For example, at national level, Li et al. [36] estimated the N_2O emission rate from the croplands of America was 0.9–1.2 Tg N yr^{-1} by using the DNDC model. Smith et al. [37] also reported the N_2O emissions from the agricultural soils of Canada. At regional scale, Li et al. [11] predicted the net GHG emissions and the increase of crop yield next 20 years in rice production areas of China. Qiu et al. [6] simulated the SOC storage in the soils of northeast China by using the validated model. Wang et al. [38] and Qiu et al. [39] reported the long-term dynamics of the SOC and the effects of different management practices on the CO_2, N_2O and CH_4 emissions in six main agricultural production areas in China by using DNDC model, respectively. Zhang et al. [35] took the country area as the minimum grid cell to simulate the CH_4 emission of paddy field in Tai Lake region by using the DNDC regional model that had been validated against the measured data. These reports all provided the basis for compiling the inventories of regional GHG emissions. Moreover, based on spatial analysis, DNDC model can quantitatively identify the regions that have high GHG emissions, and hence the proper management practices and mitigation methods suitable for each practical agricultural area can be proposed. For example, Wang and Li [17] estimated the CO_2 and NO_2 emission rates from croplands of Huang-huai-hai Plain in Hebei Province. The result showed that the winter wheat and summer maize rotation field contributed about 40% of CO_2 and N_2O emissions. And thus, the effective measures to reduce the CO_2 and N_2O emission should focus on the high CO_2 and N_2O emission regions. It might be unnecessary or not effective to reduce the CO_2 and N_2O emission at a large scale. Li et al. [40] also found that it may reduce the GHG emission in wheat–maize rotation fields in North China through increasing application of organic manure and enhancing the rate of straw residue returned to field instead of increasing chemical fertilizer application. Anyway, the DNDC model will play an important role in regional agricultural sustainable development.

5. The model development

The continuous development of a model is regarded as one of the criteria to appraise whether the model was acceptable or successful. During the past decade, along with more international researchers involved in the modeling effort, DNDC has been substantially enhanced and become a generic agro-ecosystem model for predicting crop growth, C sequestration, greenhouse gas emissions, nitrate leaching, and water use efficiency for all terrestrial ecosystems including upland, wetland, grassland, forest, etc. Zhang et al. [41] had developed Crop-DNDC model through combining the crop growth rules and the DNDC model, which can simulate soil moisture, leaf area index, the biomass of overground and underground part of crops. The improved model provided a powerful tool for evaluating comprehensive effects of climate change and management measures change on crop yield, SOC sequestration and greenhouse gas emissions. Combined the economic model CAPRI with DNDC model, Leip et al. [42] developed the CAPRI DNDC-EUROPE model, through which they simulated the GHG emissions, the changes of soil carbon storage and nitrogen balance from European agricultural soils, and also evaluated the impacts of various agricultural policies on the development of economy and society. Neufeldt et al. [43] developed an economic ecological model, EFEM–DNDC model, combining DNDC model with EFEM model, to comprehensively evaluate the influence of livestock breeding and crop cultivating on greenhouse gas emissions and economic benefits in the typical farms of southwest Germany. Cui et al. [44] linked MIKESHE model (a hydrological model) with DNDC model, with a few modifications of the input parameters and the biogeochemical process in heterotrophic conditions of the model, to evaluate the long-term change of soil carbon and greenhouse gases emissions from the wetland ecosystem, which provided a decision-making basis for future management of carbon revenue and expenditure. Stange et al. [45] added the trees growth submodel into DNDC model developing PnET-N-DNDC model, which extended the application range of DNDC model simulating soil N_2O and NO emissions from cropland ecosystem to the forest ecosystem. Based on the framework of the PnET-N-DNDC model, with the modifications including the dynamics of underground water table, soil thermal conduction, the growth of bryophytes and herbage, and various biogeochemical processes in heterotrophic conditions, Zhang et al. [46] had developed Wetland-DNDC which could be applied to the forest and wetland ecosystem. And then, combined PnET-N-DNDC and Wetland-DNDC model, they established forest-DNDC predicting the growth of plants, the dynamics of water and other elements such as C and N, especially the emissions of CO_2 and CH_4 from forest ecosystem. Also based on the framework of the PnET-N-DNDC model, by adding the new features including the impacts of water scarcity and rainstorm on crop leaves, denitrification activity index and biological nitrogen fixation algorithm, Kiese et al. [47] used the improved model to estimate the N_2O emissions of the Australian tropic rainforests. In addition, DNDC model was also developed for applying in specific environment conditions of a nation or region. For example, Brown et al. [48] developed UK-DNDC specially for the British climate and soil environment, and estimated N_2O emissions from the British agricultural soils; Saggar et al. [49] established NZ-DNDC model for New Zealand ecosystems, and simulated the N_2O emissions of New Zealand grasslands; The researchers from the Institute of Agricultural Resources and Regional Planning, Chinese Academy of Agricultural Sciences improved DNDC model suitable for a particular watershed to simulate carbon and nitrogen cycle at watershed-scale and quantitatively evaluate agricultural non-point pollution. In future, DNDC model may play more and more important role in analyzing and predicting the mutual effects between human activities and global climate change.

6. Discussions

6.1. The testing criteria for the model

The goodness of fit between simulated and measured values was the fundament for the model's further application. Therefore, it was important for the model validation, but appraising the goodness of fit between simulated and measured values cannot depend on the intuition but need strict statistical test. Usually there were many statistical metrics to assess the simulation accuracy. The two metrics most commonly used were as follows:

$$\left(U^2 = \frac{\sum_{t=1}^{N}(S(t)-O(t))^2}{\sum_{t=1}^{N}(O(t))^2}\right) \times \left(r = \frac{\sum_{t=1}^{N}(S(t)-\overline{S})\times(O(t)-\overline{O})}{\sum_{t=1}^{N}\sqrt{(S(t)-\overline{S})^2}\times\sum_{t=1}^{N}\sqrt{(O(t)-\overline{O})^2}}\right)$$

where $O(t)$ and $S(t)$ are measured and simulated values, respectively; $\overline{O}$ and $\overline{S}$ are the mean values of measured and simulated values, respectively; N is the number of data points. And U stands for *Theil Inequality coefficient*, $U = 0$ results when the best fit of the model to the observations has occurred, and $U > 1$ signifies the model performs worse; r represents correlation coefficient, An r-value closest to 1 indicates the model matches the pattern of the observations and has a perfect simulation. But the results from these formulas cannot completely evaluate simulation accuracy. For example, a report showed that the model had a good performance in simulating annual total N_2O emission rates, effects of agricultural activities, and can also capture the N_2O emission peak in the soil [40], but the model may not completely fit the time of the peak occurred, which may result in a conclusion that the model had a poor performance due to not meeting the bias criteria using the metrics assessing method. Therefore, model validation was a relatively comprehensive and complicate process, which needed not only considering the dynamic changes of the GHG emission, but also the total emission rates.

6.2. Uncertainty analysis of the model results

DNDC have already been tested against field observations accumulated worldwide, but errors still existed for using the model in a large scale. The errors were mainly from the hypothesis before we applied the model to the regional scale, namely we assumed all of the attributes in each grid cell were uniform. However, the hypothesis was not in accord with the actual situation, especially for the soil properties (e.g., texture, SOC content and pH) which were inherently heterogeneous in space. Averaging the variations of the soil properties may result in uncertainties of the model results as soil properties were key factors affecting GHG emissions. Therefore, it will reduce the model error if the grid cell was divided more accurately. For example, if the grid cell reduced from 'Country' to '1:50,000 plot', the difference of simulated CH_4 emissions from paddy soils in Tai Lake region can reach 40% [50]. Therefore, the division level of the grid cell was an important factor to guarantee the regional modeling accuracy. In addition, a simulation uncertainty was directly related to the accuracy of the input parameters required by the DNDC model. With the wide application of the model and improvement of environment parameters database, the DNDC model will continuously improve the accuracy for the region-scale simulations.

6.3. The future development of DNDC

DNDC was originally developed to simulate soil GHG emissions including N_2O, NO, CH_4 and CO_2, and to quantitatively analyze the effects of management practices on GHG emissions. Recently, we were encouraged by the recent improvement to DNDC for nitrate leaching estimation. New water retention features were added to DNDC by introducing a virtual water pool to control the tile discharge flow. And meanwhile, an adsorbed N pool was created in DNDC to simulate the buffering effect of soil on the amount of nitrate available for leaching. The Langmuir equation was adopted to simulate adsorption and desorption of ammonium ions on the soil absorbents. With these modifications, the model not only improved the prediction of water leaching fluxes in the soils, but also enhanced the capacity for simulating free ammonium dynamics, nitrification, and nitrate leaching [51]. The modified DNDC showed that the modeled impact of differences of precipitation, soil texture, soil organic carbon content, and fertilizer application rates on nitrate leaching rates were consistent with observations reported by other researchers [52], and then had been applied for simulating nitrate leaching rates in typical watershed regions in Huang-huai-hai Plain [53]. However, we realized there were still limitations for widespread application of this tool. The various environment conditions (e.g., soil heterogeneity and climate) would be the major obstacle for applying the model across sites. Therefore, if the model was applied to a new site, we suggested carrying out tests to verify or modify the model. Moreover, it still lacked validation tests of the model for GHG emissions and nitrate leaching estimation simultaneously. In future, we will continue testing the model against more observations across climate zones, soil types, and management regimes. We expect these efforts will enhance the applicability of DNDC for predicting GHG emissions, N leaching and crop yields at regional scales that are attracting more attentions across China.

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