Mathematical and computer models for predicting greenhouse gas emissions from soil into the atmosphere: review and comparison

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Abstract—**Climate change is one of the pressing global issues facing humanity. Greenhouse gases play a pivotal role in this process, as they are emitted from the soil and interact with the atmosphere, altering the climate balance. This article explores mathematical and computer models used to estimate the volumes of gas emissions from the soil, aiming to identify current and effective approaches for monitoring such emissions, taking into account land use types. Essential parameters for modeling greenhouse gas migration processes and monitoring their impact on climate change are defined.**

In this study, we undertake a comparative analysis of models used to assess this process, considering climatic conditions, soil type, and particle size distribution, is provided. The results of model comparisons can be employed to evaluate greenhouse gas emissions, study their influence on climate change, and develop strategies to combat global warming.

Keywords—greenhouse gases, carbon dioxide, soil respiration, mathematical model, information system, carbon, methane, soil organic matter.

I. Introduction

The soil environment is one of the essential conditions for the existence of living organisms on planet Earth. In this ecosystem, continuous processes of organic matter transformation take place. One of the outcomes of such processes is the emission of greenhouse gases into the atmosphere.

These gases are among the primary components that have a significant impact on climate change. As stated in [1]: "Climate change, caused by greenhouse gas (GHG) emissions, is one of the most serious threats facing our planet, and is of concern at both UK and devolved administration levels. Accurate predictions for the effects of changes in climate and land use on GHG emissions are vital for informing land use policy".

Agricultural lands serve as a source of greenhouse gas emissions. Assessing the volume of emissions of these gases is necessary for developing a strategy to maintain the balance between the natural environment and human agricultural activities. In our review study, we compare mathematical models and information systems used to predict and estimate the volumes of greenhouse gas emissions.

II. Models for Predicting Greenhouse Gas Emissions

A. Model DNDC

DNDC (DeNitrification-DeComposition) is an information system based on a mathematical model developed to assess the dynamics of carbon and nitrogen in agroecosystems, taking into account the impact of agricultural activities on climate change. This model has several modifications that can be used to estimate greenhouse gas emissions in agroecosystems, mountainous and wetland forest ecosystems, pastures, and livestock farms. It describes the interaction between soil, plants, and the atmosphere and considers processes related to the emissions of greenhouse gases such as carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), nitric oxide (NO), dinitrogen (N_2), and ammonia (NH_3).
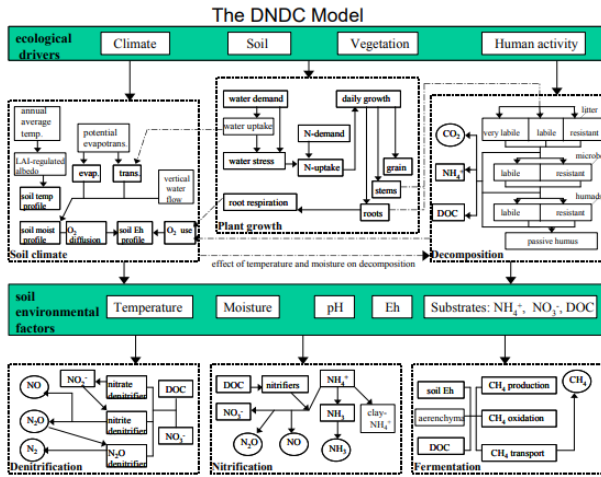
Figure 1.   Model Structure [3, p. 8]

The DNDC model also describes the impact of agricultural practices on carbon dioxide sequestration, models daily plant growth and crop yield, simulates the migration of nutrients in the soil environment, and their uptake by plants.

To calculate greenhouse gas emissions in the DNDC model, data on soil type, climatic conditions, and land use methods are also employed. According to the statement in [4]: "The model uses the parameters of heat transfer rate, specific heat capacity, and thermal conductivity of soil to calculate soil temperature layer by layer and balances the relationship of input water and output water to calculate the soil moisture of each layer".

The change in carbon (C) and nitrogen (N) quantities in the model varies relative to their amounts in the aboveground ecosystem. The model takes into account the influence of moisture and temperature at different soil depths.

The primary sources of greenhouse gas generation and absorption include processes such as organic residue decomposition, nitrification, denitrification of nitrogen, and fermentation, which leads to methane production.
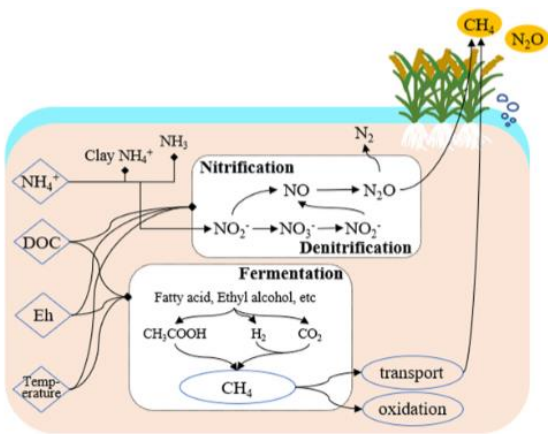

Figure 2.   The scheme of greenhouse gas emission process in the DNDC model[4, p.143]

B. Model DAMM

DAMM (Dual Arrhenius and Michaelis–Menten Kinetics Model) is a mathematical model based on the Michaelis–Menten equation. This equation describes the rate of enzymatic reactions as a function of the concentration of an organic substrate.

In this model, various sources of substrate input and microorganisms that transform it can be incorporated.
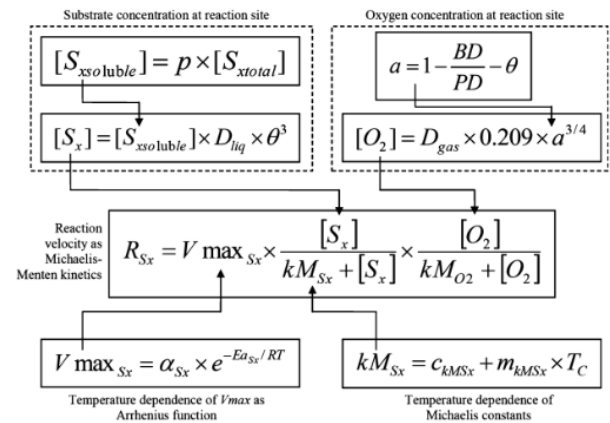

Substrate concentration at reaction site

$$[S_{xsoluble}] = p \times [S_{xtotal}]$$

$$[S_x] = [S_{xsoluble}] \times D_{liq} \times \theta^3$$

Oxygen concentration at reaction site

$$a = 1 - \frac{BD}{PD} - \theta$$

$$[O_2] = D_{gas} \times 0.209 \times a^{3/4}$$

Reaction velocity as Michaelis-Menten kinetics

$$R_{Sx} = V\max_{Sx} \times \frac{[S_x]}{kM_{Sx} + [S_x]} \times \frac{[O_2]}{kM_{O2} + [O_2]}$$

$$V\max_{Sx} = \alpha_{Sx} \times e^{-Ea_{Sx}/RT}$$

Temperature dependence of $Vmax$ as Arrhenius function

$$kM_{Sx} = c_{kMSx} + m_{kMSx} \times T_C$$

Temperature dependence of Michaelis constants

Figure 3.   Graphical representation of the DAMM model [5, p.372]

According to article [6]: "In its current form, it would not be suitable for several potentially important applications, such as permafrost thaw or methane fluxes. Most importantly, it only addresses fast-response soil heterotrophic respiration processes and is not yet connected to processes related to C inputs or to C stabilization".

The DAMM (Dual Arrhenius and Michaelis–Menten Kinetics Model) takes into account the influence of temperature, soil moisture, and the concentration of soluble substrates on the transformation of organic carbon substrates in the soil. The concentrations of dissolved carbon and oxygen in the soil are modeled using diffusion equations. Since the model considers oxygen, it can be applied to simulate aerobic respiration, which is most common in mountainous soils. This model can also be modified as needed.

C. Model DETECT (DEconvolution of Temporally varying Ecosystem Carbon componenTs)

This is a mathematical model of physical processes for predicting, generating, and migrating carbon dioxide in the soil environment based on depth and time. The model considers that carbon dioxide is generated as a result of root respiration, as well as the activities of associated microorganisms and microbial processes.
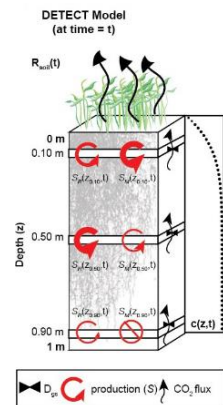
Figure 4.   Graphical representation of DETECT model components[7, p.1912]

Effective diffusion of carbon dioxide through the soil is assumed to be the same for CO2 originating from roots and microorganisms. The model assumes that CO2 transport in the soil profile occurs through diffusion mechanisms. According to article [7]: "Although DETECT v1.0 assumes that root and microbial respiration are independent of one another, they both depend on the same environmental data".

The maximum potential decomposition and respiration rates of free-living soil microorganisms vary with depth and time, unlike DAMM (which does not vary with depth). The model accounts for both the dissolved and microbial carbon pools and is relevant for systems not limited by the presence of oxygen.

Soil temperature and moisture are calculated using a separate HYDRUS model [18]. The model considers that previous temperature and moisture levels influence the formation of carbon dioxide. The decomposition process in the DETECT model is described by Michaelis–Menten kinetics.

The model does not consider diffusion in the liquid phase, convection, or transportation through vertical water movement.

D. Model DAYCENT (Daily Century)

The DAYCENT (Daily Century) model is a mathematical model described by a dynamic system and is used to predict the dynamics of biogeochemical processes in ecosystems, including carbon dioxide emissions from the soil. This model is developed based on the CENTURY model with a daily time step and accounts for more complex processes such as nitrogen leaching and the presence of soil carbon in various forms. The model consists of submodels that assess nitrogen and carbon fluxes, plant productivity, organic residue decomposition, soil water dynamics, and temperature.

According to article [9]: "DAYCENT simulates exchanges of carbon, nutrients, and trace gases among the atmosphere, soil, and plants as well as events and management practices such as fire, grazing, cultivation, and organic matter or fertilizer additions".

DAYCENT simulates the emissions of nitrogen gases resulting from nitrification and denitrification processes.
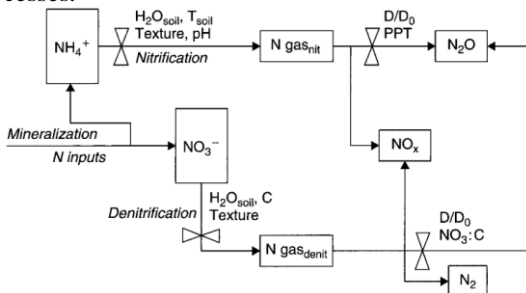
Figure 5.   Diagram of the N gas flux submodel in the DAYCENT model [9, p.575]

The model also assesses methane and carbon emissions from the soil environment. According to the statement in [10]: "Total C flow out of the active pool is

a function of potential decomposition rates modified by the effect of moisture, temperature, pH, and soil texture".

E. Model PaSim (Pasture Simulation Model)

As stated in [11]: "PASIM is a biogeochemical grassland ecosystem model that simulates fluxes of C, N, water, and energy at the soil-plant-atmosphere interface, as well as net primary productivity and forage intake by domestic herbivores".
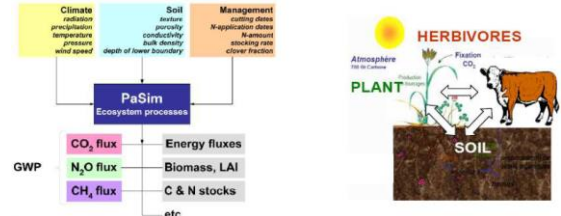
Figure 6.   Model Schema of PaSim [11, p.1]

When modeling the ecosystem, factors such as soil carbon content, plant organic matter content, and nutrient levels are taken into account.

In PaSim, three sources of carbon dioxide formation are considered: autotrophic respiration, organic residue decomposition, and heterotrophic respiration. It accounts for nitrogen processes such as mineralization, nitrification, and denitrification.

Carbon content is influenced by the dynamics of changes in the quantity and quality of plant biomass in pastures. Additionally, the model considers the impact of pasture management practices (such as different fertilization methods and forage harvesting) on the carbon balance.

PaSim has limitations regarding modeling high temperatures and severe droughts.

F. Model ECOSSE

The mathematical model ECOSSE (Ecosys Climate Change Soil Emission model) simulates the impact of land use on climate change, greenhouse gas emissions, carbon and nitrogen stocks in soils, and models the process of organic matter biodegradation.

According to the statement in [13]: "The ECOSSE model was developed to simulate highly organic soils from concepts originally derived for mineral soils in the RothC and SUNDIAL models".

The model takes into account that during aerobic decomposition of organic residues, carbon dioxide is emitted, while under anaerobic conditions, methane is produced. To enhance the accuracy of simulating soil processes, the model divides the soil into layers of 5 cm each.
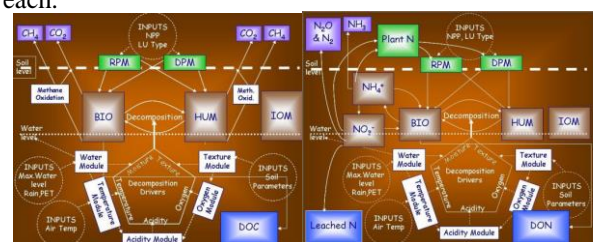
Figure 7.   Model Schema (Structure of Carbon and Nitrogen Components of the Model) [13, p.12]

In the model, each layer is considered a homogeneous unit that produces carbon dioxide under aerobic conditions. Additionally, emissions of nitrogen

resulting from denitrification and partial nitrification are also simulated.

III. CONCLUSIONS

Therefore, mathematical and computer models for predicting greenhouse gas emissions contain the following components: modeling the thermal state of the soil, modeling the moisture state of the soil, modeling biological processes, modeling the influence of anthropogenic factors, and modeling the interaction between plants and soil.

Each of the models discussed has its own specific features and advantages that can be utilized for the determination and prediction of greenhouse gas emissions from the soil.

Considering the diversity of the models discussed, it is important to take into account the initial dataset and the forecasting objectives before selecting a specific model.

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