Soil carbon and nitrogen mineralization: Theory and models across scales

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ABSTRACT

In the last 80 years, a number of mathematical models of different level of complexity have been developed to describe biogeochemical processes in soils, spanning spatial scales from few μm to thousands of km and temporal scales from hours to centuries. Most of these models are based on kinetic and stoichiometric laws that constrain elemental cycling within the soil and the nutrient and carbon exchange with vegetation and the atmosphere. While biogeochemical model performance has been previously assessed in other reviews, less attention has been devoted to the mathematical features of the models, and how these are related to spatial and temporal scales. In this review, we consider ~250 biogeochemical models, highlighting similarities in their theoretical frameworks and illustrating how their mathematical structure and formulation are related to the spatial and temporal scales of the model applications. Our analysis shows that similar kinetic and stoichiometric laws, formulated to mechanistically represent the complex underlying biochemical constraints, are common to most models, providing a basis for their classification. Moreover, a historic analysis reveals that the complexity and degree and number of nonlinearities generally increased with date, while they decreased with increasing spatial and temporal scale of interest. We also found that mathematical formulations specifically developed for certain scales (e.g., first order decay rates assumed in yearly time scale decomposition models) often tend to be used also at other spatial and temporal scales different from the original ones, possibly resulting in inconsistencies between theoretical formulations and model application. It is thus critical that future modeling efforts carefully account for the scale-dependence of their mathematical formulations, especially when applied to a wide range of scales.

1. Introduction

About three-fourth of the organic carbon contained in terrestrial ecosystems and the majority of organic nitrogen are found in plant residues and soil organic matter (Schlesinger, 1997; Lal, 2008). Both organic carbon and macro-nutrients are mineralized to simple inorganic forms by a highly dynamic community of microbial and faunal decomposers (Brady and Weil, 2002; Berg and McClaugherty, 2003; Paul, 2007). Although this process of mineralization occurs at the decomposer cell scale and is affected by the soil physical and biological interactions (e.g., climate and vegetation), it involves globally a gross release of carbon dioxide to the atmosphere in amounts one order of magnitude larger than the anthropogenic emissions (Schlesinger, 1997; Lal, 2008) and provides most of the inorganic nutrients necessary for plant growth in natural ecosystems (Waksman et al., 1928; Brady and Weil, 2002).

Since the 1930s, several mathematical models at different levels of detail have been developed to quantitatively describe these processes (e.g., Tanji, 1982; Dewilligen, 1991; McGill, 1996; Molina and Smith, 1998; Benbi and Richter, 2002; Shibu et al., 2006). The number and variety of these models mirror a relentless effort to describe and quantify the complex nature of soils and the elemental cycling within them. Soils are spatially heterogeneous at molecular to continental scales (Ettema and Wardle, 2002; Young and Crawford, 2004), and their temporal dynamics span a wide range of scales going from the hourly responses to environmental fluctuations (Austin et al., 2004; Schwinning and Sala, 2004) and changes in resource supply (Zelenev et al., 2000), to the decadal time scales of ecosystem and climatic changes and the even longer time scales characteristic of soil development (Richter and Markewitz, 2001). The extreme variety of biogeochemical processes is further complicated by climatic and anthropogenic external forcing factors.

The development of a mathematical model generally follows three subsequent steps (Ulanowicz, 1979): i) definition of the state

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variables for the scale of interest; ii) identification of inputs, outputs, and possible interactions; iii) model verification. Most of the previous reviews on biogeochemical modeling primarily address the verification step (e.g., Dewilligen and Neeteson, 1985; Andrén and Paustian, 1987; Melillo et al., 1995; Powlson et al., 1996; Jans-Hammermeister and McGill, 1997; Smith et al., 1997; Moorhead et al., 1999; Zhang et al., 2008). Fewer works focus on the first two critical steps: describing the effects of different choices of the state variables (e.g., Bolker et al., 1998; Bruun et al., 2004; Pansu et al., 2004; Fontaine and Barot, 2005) and comparing different formulations of the interactions among them (Molina and Smith, 1998; Ma and Shaffer, 2001; McGechan and Wu, 2001; Plante and Parton, 2005; Manzoni and Porporato, 2007; Wutzler and Reichstein, 2008).

The goal of this review is not to test modeling hypotheses or assess model performances, but to provide an extensive comparison of mathematical approaches to soil carbon (C) and nitrogen (N) cycling and discuss a model classification based on kinetic laws and stoichiometry. The difficulty of classifying soil biogeochemical models according to their mathematical formulation arises because of the large number of possible combinations of different model structures (e.g., number of variables and mass flow architecture) and reaction terms (e.g., linear vs. nonlinear kinetic laws). However, all these models deal with processes controlled by similar biogeochemical constraints, and basically describe the transfer of matter from organic to inorganic compounds. This mineralization process can be regarded as a complex, biologically mediated series of reactions, where organic substrates are converted into living biomass and mineral residues (Swift et al., 1979). It is typically modeled by kinetic laws describing organic matter degradation, where microbial stoichiometric relationships are employed to regulate the associated C–N balances. In what follows we will compare the mathematical formulations used to describe these two fundamental aspects of C and N cycling, with the hope to highlight possible limitations of current approaches and help future cross-disciplinary theoretical developments.

A simplified mathematical representation of the substrate–microbial biomass interactions will be presented and guide our model classification, where indices of model structure and complexity are included, along with a characterization of key biogeochemical processes (Table A2). About 250 mathematical models developed during nearly eight decades are reviewed, considering both highly cited sources and less known theoretical analyses describing the various aspects of soil dynamics, as well as soil organic matter submodels embedded in hydrologic or ecosystem models. Since model structure and formulations are expected to change with the scale and level of resolution needed for the particular applications (Manzoni and Porporato, 2007; Manzoni et al., 2008b), we also analyze the relationships between model formulations and the temporal and spatial scale of application.

The review is organized as follows:

- Section 2 describes the general structure of soil biogeochemical models, with an emphasis on stochastic components, mathematical formalisms, and level of complexity (e.g., the dimension of the phase-space), and relates these features to the scales of interest.
- Section 3 presents an overview of the mathematical formulations used to characterize two key processes in C and N cycling in soils, i.e., decomposition of organic matter and nitrogen mineralization and immobilization. Both processes are analyzed under the common framework of substrate–decomposer stoichiometry, thus stressing the role of the microbial biomass as both an SOM degrading agent and as a controlling factor of N cycling. This approach allows us to

compare mathematical models coming from different fields, ranging from microbiology to ecosystem ecology.
- Section 4 analyzes the relationships between model formulation and scale, discussing how the different formulations are used across or at individual scales.
- Section 5 puts the previous analyses into perspective with respect to the dominant trends in soil biogeochemical modeling and discusses the main limitations of the current approaches. Based on these conclusions, we provide some guidelines for future research.
- Finally, Appendix A reports the list of the reviewed models and their most important mathematical features with respect to this synthesis.

2. Historic appraisal of mathematical structure and complexity in soil biogeochemical models

Soil biogeochemical models describe a system including SOM constituents (both passive substrates and active biological decomposers), interacting with inorganic compounds, environmental variables, and subject to external inputs and outputs (Fig. 1). Here we review how the mathematical description of such a complex system is framed. We discuss the general model structure and spatial resolution (Sections 2.1–2.3), the number of variables used at different scales (Sections 2.4 and 2.5), and the presence of stochastic elements (Section 2.6).

2.1. From compartment to continuum-quality models

Although SOM is an extremely heterogeneous mixture of compounds (Swift et al., 1979), early mathematical models described the processes of decomposition and mineralization using simple chemically and spatially lumped models (Table A2; Fig. 2a). Nikiforoff (1936) was probably the first to suggest that the formation of humus may be described by multiple coupled equations each characterizing a pool with different turnover times. Later, Minderman (1968) developed similar ideas to describe the macroscopic patterns of organic matter degradation resulting from the compound effects of different substrates. This idea resulted in a number of compartmental models. As noted by Halfon, "Compartmental analysis is a phenomenological and macroscopic approach for modeling a physicochemical process. A compartment (or state variable [...]) is a basic unit of functional interest" (Halfon, 1979, p. 2). Recent models employ a number of such chemically homogeneous compartments, which interact among them and possibly with the microbial biomass (Fig. 1). Most soil food web models are also compartment models, where particular attention is given to the trophic interactions among microbial and faunal groups (Hunt et al., 1987; Deruiter et al., 1993; Zheng et al., 1999; Zelenev et al., 2006).

In compartment models, all the organic matter molecules with similar chemical characteristics or degradability are included in the same pool and the information regarding the age or residence time of biogeochemical compounds within each compartment (or in general since the introduction of organic matter into the soil system) is not explicitly tracked. Nevertheless, the distribution of the ages of SOM compounds can be reconstructed knowing the model structure and how the fluxes among the pools are defined (Bruun et al., 2004; Manzoni et al., in preparation). In contrast to typical compartment models, some biogeochemical models explicitly track the evolution of any organic matter "cohorts" (i.e., "sets of items of the same age", Gignoux et al., 2001) from their incorporation into the litter or humus and until their complete degradation (Furniss et al., 1982; Pastor and Post, 1986; Ågren and