Environmental Modelling & Software 71 (2015) 39–45

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

Short communication

Individual-based modeling of soil organic matter in NetLogo: Transparent, user-friendly, and open

Thomas Banitz [a, *], Anna Gras [b], Marta Ginovart [c]

[a] Department of Ecological Modelling, UFZ – Helmholtz Centre for Environmental Research, Permoserstr. 15, 04318, Leipzig, Germany
[b] Department of Agri-Food Engineering and Biotechnology, Universitat Politècnica de Catalunya, Campus Baix Llobregat, Esteve Terradas 8, 08860, Barcelona, Spain
[c] Department of Applied Mathematics III, Universitat Politècnica de Catalunya, Campus Baix Llobregat, Esteve Terradas 8, 08860, Barcelona, Spain

ARTICLE INFO

Article history:
Received 10 July 2014
Received in revised form
17 April 2015
Accepted 24 May 2015
Available online 13 June 2015

Keywords:
Individual-based model
Soil organic matter
Soil microorganisms
Mineralization
Nitrification
NetLogo

ABSTRACT

Soil organic matter dynamics are essential for terrestrial ecosystem functions as they affect biogeochemical cycles and, thus, the provision of plant nutrients or the release of greenhouse gases to the atmosphere. Most of the involved processes are driven by microorganisms. To investigate and understand these processes, individual-based models allow analyzing complex microbial systems' behavior based on rules and conditions for individual entities within these systems, taking into account local interactions and individual variations. Here, we present a streamlined, user-friendly and open version of the individual-based model INDISIM-SOM, which describes the mineralization of soil carbon and nitrogen. It was implemented in NetLogo, a widely used and easily accessible software platform especially designed for individual-based simulation models. Including powerful means to observe the model behavior and a standardized documentation, this increases INDISIM-SOM's range of potential uses and users, and facilitates the exchange among soil scientists as well as between different modeling approaches.

Software availability

Name of software: INDISIM-SOM-NL
Developers: Thomas Banitz, Anna Gras, Marta Ginovart
Contact e-mail: thomas.banitz@ufz.de
Available since: 2015
Software required: NetLogo 5.0 (Wilensky, 1999; http://ccl.northwestern.edu/netlogo/)
Availability: Appendix B. Model files
Cost: Free
Program language: NetLogo
Program size: ca. 100 kB

1. Introduction

Although soil science has considerably advanced during the last decades, many soil processes still remain poorly understood and, given their general importance for life on earth and human societies, urgently require further investigation (Baveye et al., 2011). For instance, the dynamics of soil organic matter (SOM) have a fundamental impact on the functioning of terrestrial ecosystems and belong to the most important factors affecting soil quality and fertility (Gabriel, 2010). Many of the involved processes are significantly influenced by soil colonizing microorganisms. Decomposing SOM into organic and inorganic carbon (C) and nitrogen (N), and also synthesizing important SOM components, microorganisms substantially contribute to the soils' C and N cycles (Grant et al., 1993; Schmidt et al., 2011). Their decomposition of SOM and mineralization to inorganic compounds also provides a substantial source of inorganic nutrients and is, therefore, a key driver of plant growth (Chen et al., 2003). Moreover, the release of carbon dioxide and nitrous oxide from soils is strongly driven by the activity of microorganisms and their interactions with environmental factors such as soil composition or temperature. The high relevance of these phenomena motivates detailed studies of the processes that govern microbial activity and the fate of C and N associated with organic matter in soils, such as metabolism of different substrates, growth and decay of microbes, hydrolysis, (de)sorption and diffusion of abiotic compounds.

Abbreviations: C, carbon; N, nitrogen; SI, super-individual(s).

* Corresponding author. Tel.: +49 341 2351708; fax: +49 341 2351473.
E-mail address: thomas.banitz@ufz.de (T. Banitz).

http://dx.doi.org/10.1016/j.envsoft.2015.05.007
1364-8152/

Mathematical models that describe these processes can contribute significantly to increase our understanding of their interactions and the resulting SOM dynamics in response to varying environmental factors. They allow for disentangling the complexities of interacting mechanisms, systematically varying biotic and abiotic conditions, and testing alternative hypotheses to explain observed phenomena. Such models have been applied for this purpose since several decades already (cf. Manzoni and Porporato, 2009 for a comprehensive review). More recently, the recognition of the importance of spatial explicitness and individual variations in microbial ecosystems has particularly favored the development of individual-based models (IBMs; Ferrer et al., 2008; Hellweger and Bucci, 2009). These bottom–up models describe an ecosystem via the behavior of micro scale components (individuals), which are often much better understood than the whole system. Then, the system behavior emerges in the model from the interactions of the individuals with each other and with the environment, as it does in reality (Grimm and Railsback, 2005). In contrast to many other mathematical models, this intuitive approach is well-suited to model highly complex dynamics based on simpler rules and assumptions, and to include local interactions, individual variability and adaptive behavior (Grimm, 2008). Nonetheless, there are also challenges, as the easily increasing complexity (Grimm and Railsback, 2005; Crout et al., 2009), the less developed conceptual and theoretical framework (Grimm and Railsback, 2005), limited programming knowledge (Lorek and Sonnenschein, 1999) or high computational demands (Devillers et al., 2010) may hinder an efficient usage of IBMs.

In line with the development towards including individual and spatial variations also in microbial models, the first IBM for SOM dynamics was presented in 2005 (INDISIM-SOM; Ginovart et al., 2005). This model is a descendant of the INDISIM model family (Ginovart et al., 2002). It describes the activity of two different metabolic types of microorganisms represented by individuals (heterotrophic decomposers and autotrophic nitrifiers) in mineral soils represented by a spatially explicit environment, and comprises a set of biotic and abiotic reactions that determine the fate and interactions of these microbes and, eventually, their influence on short-term dynamics of C and N. In this respect, the individual-based approach was favored over a macro scale model, because it does not require additional prior knowledge about the overall impact of the micro scale processes on these SOM dynamics. The IBM was confronted with experimental data and the validity of alternative mechanisms for the different components of microbial activity tested (Ginovart et al., 2005).

Aiming at increasing the explanatory (and potentially also predictive) power of the INDISIM-SOM model, comprehensive efforts were put on parameterization and sensitivity analysis, taking into account a broader experimental data set. Two studies focusing on abiotic (Gras et al., 2010) and biotic parameters (Gras et al., 2011) resulted in a very good agreement of the model output to experimental measurements. The conclusions from these studies suggested certain model simplifications (e.g. unifying the initial partitioning of abiotic SOM into different compound pools) and opened the perspective for coupling it to other models (e.g. pore scale models of solute and water transport in order to appropriately describe the effect of micro scale heterogeneities on soil C and N dynamics; cf. Baveye, 2010). These studies, however, also indicated that crucial requirements for further developing the model and increasing its application potential are the confrontation to more experimental data and the consideration of additional or different micro scale mechanisms (Gras et al., 2010, 2011).

Here, we contribute to fulfilling these requirements by presenting a novel streamlined version of the model, named INDISIM-SOM-NL. In addition to model simplifications, this new version drastically facilitates exploring the effects of microbial behavior and abiotic factors on SOM dynamics (e.g. for didactical purposes), and allows soil scientists to test their own (virtual or measured) initial and parameter values or to confront the model output to own observational data.

Former INDISIM-SOM versions had been implemented in the Fortran programming language. In spite of computational efficiency and other benefits, this may often impose a substantial barrier for scientists not familiar with developing computer programs using general purpose languages (Sierra et al., 2012). Therefore, INDISIM-SOM-NL was implemented in the widely used, free and open source IBM software platform NetLogo (Wilensky, 1999; Fig. 1). This provides full access to the simulation model, including a graphical user interface and the model's source code. Given NetLogo's rather flat learning curve and comprehensive documentation (Railsback and Grimm, 2012), also users without extensive modeling experience may modify the code and, thus, investigate alternative mechanisms or adapt certain processes according to a particular study focus (e.g. introducing temperature effects, variations in soil porosity or moisture, among others).

2. Novelties of INDISIM-SOM-NL

INDISIM-SOM-NL is a revised version of the former individual-based model for SOM dynamics INDISIM-SOM. Hence, we provide an overview of the model processes (Fig. 2), and highlight in brief the modifications in comparison to recent implementations (Gras et al., 2010, 2011). The reader is referred to these studies for a detailed description of the microbiological justifications of the model structure, assumptions and processes. Moreover, we provide a complete standardized model description (Supplement A.1) following the ODD (Overview, Design concepts, and Details) protocol for describing individual-based models (Grimm et al., 2006, 2010). Additional instructions on how to use and modify the model are included in the INDISIM-SOM-NL software (in the *Info* tab, Appendix B).

The graphical user interface (Fig. 1) allows changing the variable initial values (cf. Supplement A.2). Moreover, it provides direct observations of the modeled system dynamics. This includes visualizations, such as plots of all modeled compounds, certain pools of compounds (e.g. C in labile compounds, mineralized N) and microbial C over time, biomass distributions of super-individuals (SI, individuals corresponding to a fixed larger number of microbes) for both metabolic groups, as well as spatial distributions of each compound and of SI. Further, monitors of SI numbers, microbial C, organic C and N, and total C and N are provided (cf. Fig. 1, Supplement A.1.4, Table A.4). Based on this multitude of observations at different levels, users can directly explore the consequences of changing initial or parameter values, better understand the interactions of modeled mechanisms, and immediately compare the emerging results to expected or measured behavior. To save computation time when focusing on a broader analysis of the sensitivity to certain initial/parameter values or to stochastic variations (e.g. using NetLogo's BehaviorSpace), these observations can be switched off and output text files used instead.

The new model is programmed using mass units (grams) instead of amount of substance units (moles) to express compound and microbial biomass quantities. This supersedes transformations before analyzing and interpreting those quantities in the model, and facilitates using experimental data, which are typically given in mass units. Yet, the kinetic reactions given in the preceding studies were maintained (e.g. for microbial growth or hydrolysis, Supplement A.1.7).

The previous model versions included three specific sets of coefficients for the partitioning of initial organic C and N into