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

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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.

Highlights

We present a NetLogo version of an established IBM of SOM dynamics driven by microbes.

The model was made simpler and less specific to increase its application potential.

Users may easily access, explore and also modify the computational model.

We provide the first complete standardized model description of INDISIM-SOM.

The overall aim is an improved understanding of carbon and nitrogen dynamics in soils.

Keywords

Individual-based model; Soil organic matter; Soil microorganisms; Mineralization; Nitrification; NetLogo

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.

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).

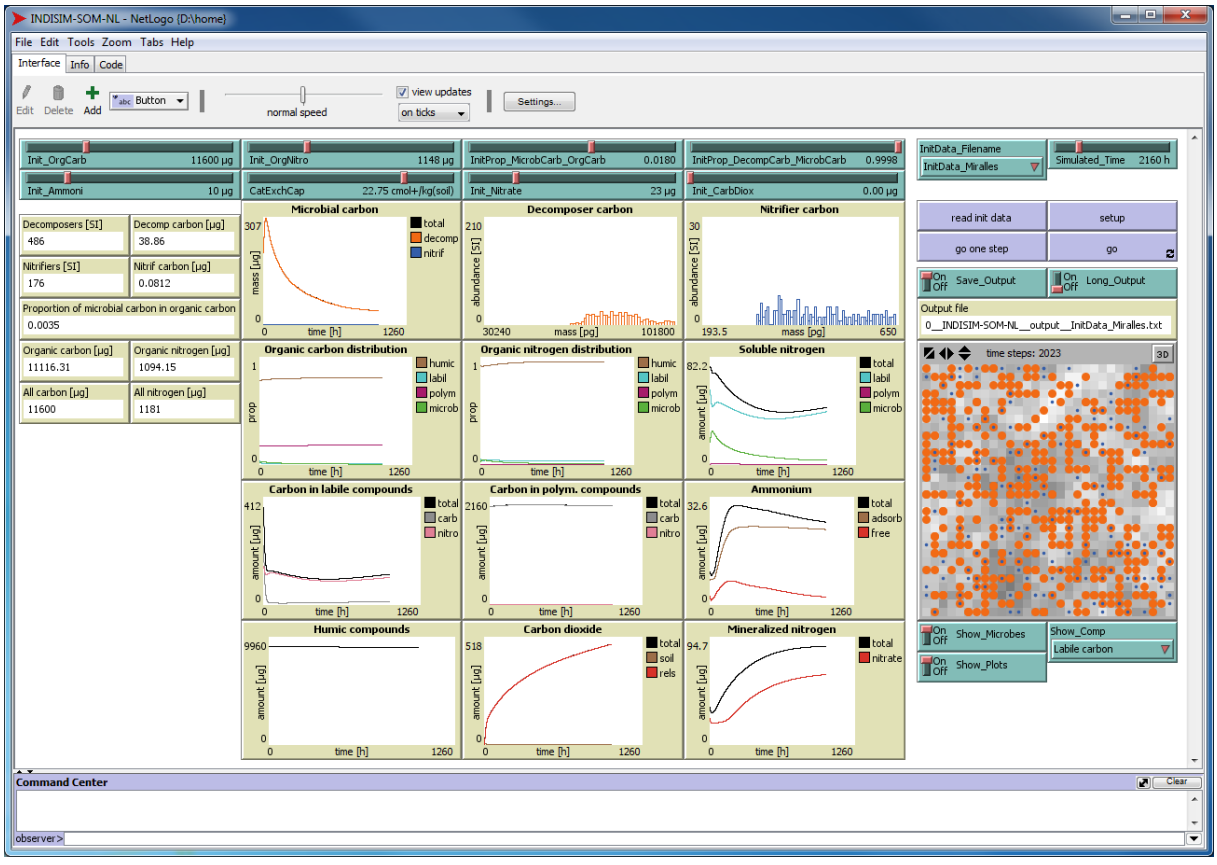
Aiming at increasing the explanatory (and potentially also predictive) power of the INDISIM-SOM model, comprehensive efforts were put on parameterization and sensitivity analysis, taking into account a broader experimental data set. Two studies focusing on abiotic (Gras et al., 2010) and biotic parameters (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).

Figure 1. INDISIM-SOM-NL user interface. The sliders in the upper part allow changing initial values and simulated time. Alternatively, the initial values are read from a file using the chooser and button in the upper right part. The remaining buttons setup and run the simulation. Below these buttons, the text file output can be specified. Observations are provided with monitors (left), plots of microbial biomass distributions and of modeled compounds over time (center), and the grid cell representation of the modeled environment (right). Below these grid cells, the user selects which compound's spatial distribution is plotted and whether or not microbe super-individuals and compound plots are shown. For further details, see the full model description (Supplement A.1).

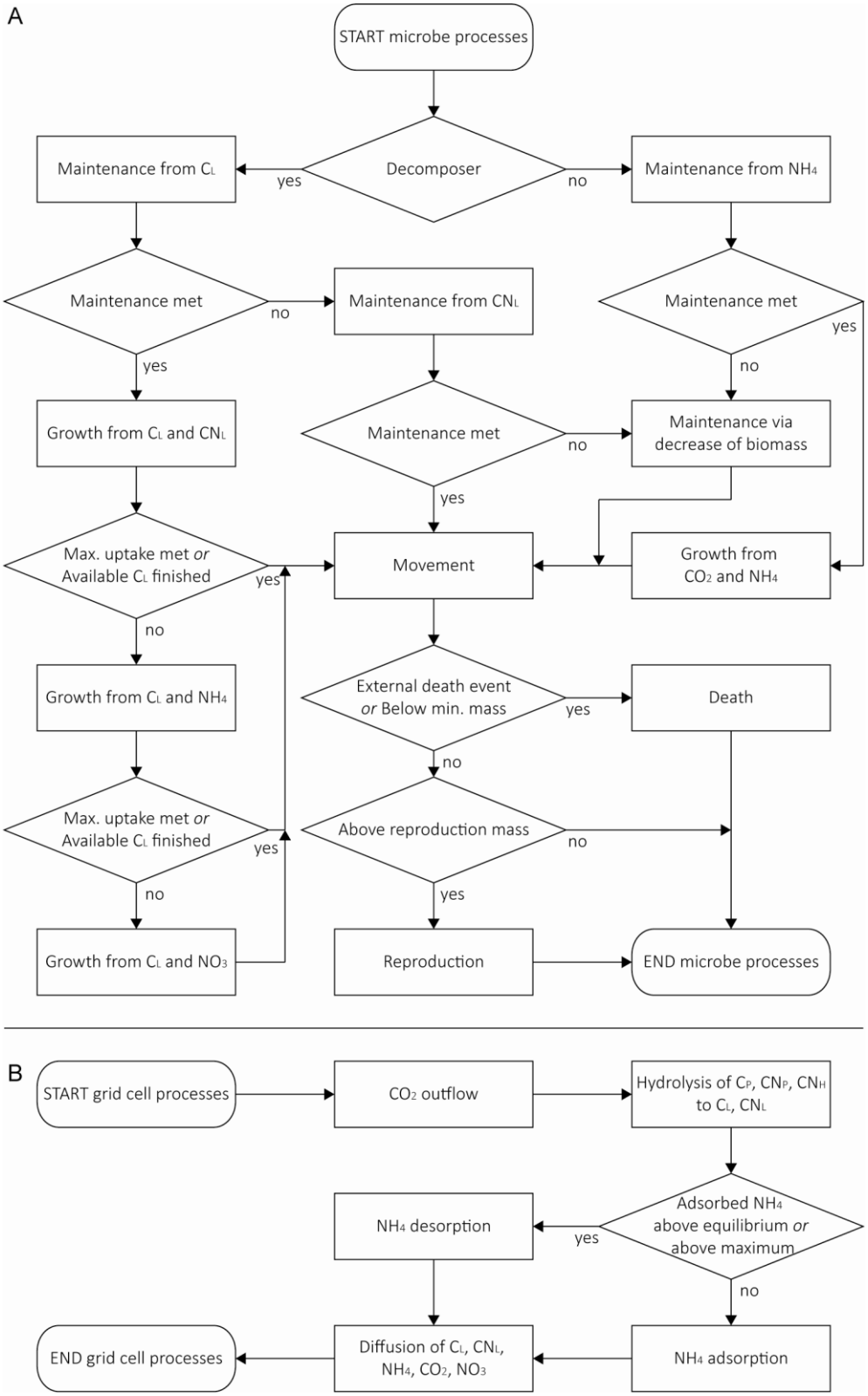


2. Novelties of INDISIM-SOM-NL

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.

Figure 2. Overview of the model processes and scheduling, see Supplements A.1.3 and A.1.7 for details. The flow charts show the processes comprised in one time step for each microbe super-individual (A) and each grid cell of the environment (B).



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 microbial biomass and different abiotic compound pools, for three different soil types (from the locations Calaf, Miralles and Caldes in Catalonia, Spain; cf. Gras et al., 2010). Here, we developed a unified partitioning scheme for the abiotic compounds (steps (e)-(j) in Supplement A.1.5). To this end, we fixed the parameter values for the initial proportions of humic and polymerized compounds in organic N and in organic C ($p^0_{CN_H}$, $p^0_{CN_P}$ and $p^0_{CN_H+C_P}$, Table A.2) based on the recent parameterization, which had shown little or no variation in these values among the three soil types (Gras et al., 2010). This unification allows simulating also different initial conditions in terms of organic N and C for soil types of similar composition without additional parameterization efforts or explicit knowledge of the specific partitioning into the abiotic compound pools. If this knowledge is available for a certain soil type, however, it will be possible to modify the model's partitioning scheme and adjust it to experimental measurements (cf. Section 3). The specific differences in the initial proportions of microbial biomass in organic C (p^0_{mic} , step (a) in Supplement A.1.5) were maintained, as they had shown significant variation among the three soil types after fitting to experimental observations (from 0.015 to 0.025; cf. Gras et al., 2010).

In previous model versions, the total microbial biomass' effects on external death events and hydrolysis (global density effects) were related directly to the initial proportion of

microbial C in organic C (Gras et al., 2010). Here, we defined a fixed reference amount of microbial C to be used instead (p^*_{mic} , Supplement A.1.7). This avoids effective microbial death probabilities and kinetic constants for hydrolysis being extremely sensitive to the initial microbial biomass, and increases the model's robustness to user modifications of the initial conditions (in terms of microbial C or organic C and N, Supplement A.1.5, cf. Fig. 1).

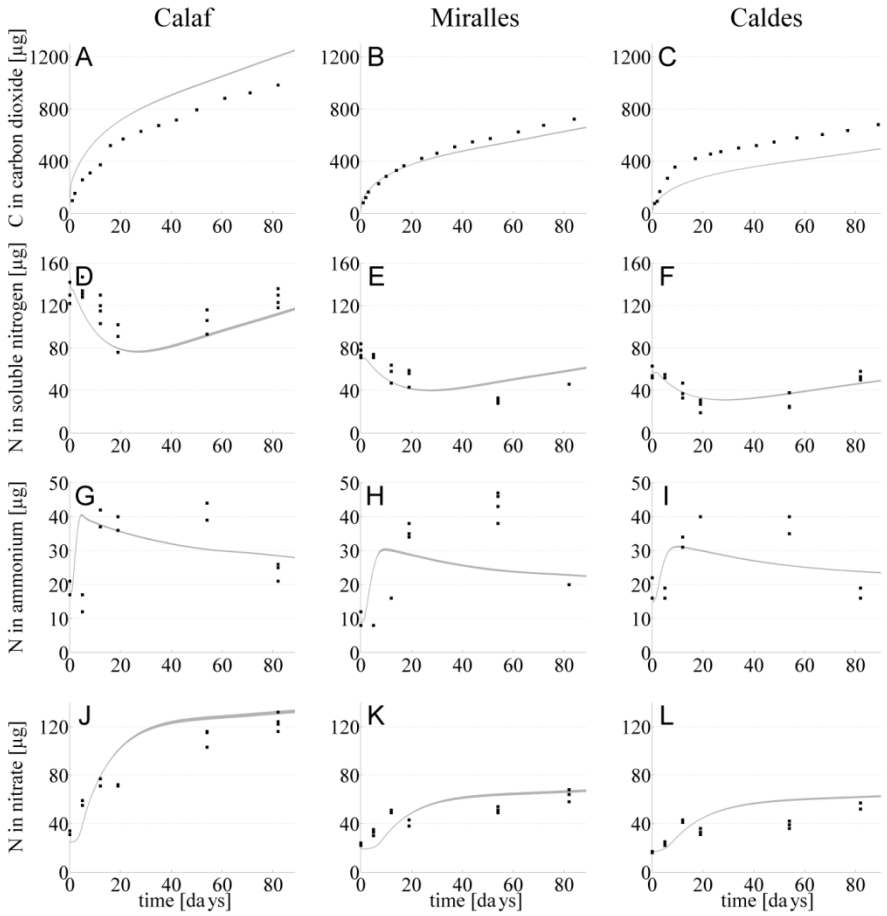
The model describes SOM dynamics in top soil. In former versions, the grid cells were constantly aerated. This maintained oxygen concentrations at atmospheric level in the soil's gaseous phase, prevented anaerobic environmental conditions in the liquid phase, and led to marginal oxygen limitation of the microbial metabolism occurring only in the beginning of the simulations (Gras et al., 2010; 2011). Here, we therefore dispensed the representation of oxygen, thus simplifying the model processes maintenance and growth (Supplement A.1.7). However, reintroducing oxygen is possible without modifying the model's general structure. Thus, limitations arising from reduced oxygen inflow and also anaerobic microbial metabolism (soil denitrification) can be taken into account in future studies. Nonetheless, it should be kept in mind that the causes of anaerobic conditions may have additional effects on the model processes or environmental characteristics.

As a consequence of the novel partitioning scheme and global density effects, and the omission of oxygen, the model's emergent system dynamics changed slightly. Therefore, we fitted the model parameter values again to the data measured in three different soil types (cf. above). We followed the previously described method of trial and error adjustments based on expert knowledge (Gras et al., 2010). The eventually changed parameter values are the kinetic constant for hydrolysis of polymerized nitrogen (Table A.2) and the availability proportions of liquid phase compounds (Table A.3). Overall, a reasonable agreement between simulated and observed carbon dioxide, soluble N and mineralized N dynamics was achieved (Fig. 3). In particular for carbon dioxide, this agreement is not as high as in previous parameterizations

with different soil type specific partitioning coefficients (Gras et al., 2010; 2011). However, developing INDISIM-SOM-NL we did not give priority to perfect reproduction of the experimental data, but to a simpler and more general model of SOM dynamics driven by microbes interacting with their abiotic environment.

Additionally, we analyzed the new model version's sensitivity to the time step length and the super-individual (SI) size (i.e. the fixed number of microbes comprised in each SI; cf. Scheffer et al., 1995). In general, shorter time steps and smaller SI favor the advantages of IBM, particularly because the higher resolution reduces averaging or ignoring the effects of local interactions and individual variations (Grimm and Railsback, 2005). However, it comes at the cost of higher computation times (Scheffer et al., 1995), which is unfeasible for quickly performing and observing simulations with INDISIM-SOM-NL. We determined an appropriate trade-off between model resolution and computation efficiency at a time step length of 30 min and SI corresponding to either 5E5 decomposer or 5E3 nitrifier microbes (Supplement A.3). Nonetheless, the model code is prepared for changing these two parameter values, such that users may test several resolutions and eventually also perform specific sensitivity analyses for different initial conditions.

Figure 3. Measurement data (black squares) and INDISIM-SOM-NL simulation results (mean values of 20 simulation runs plus/minus the standard deviations, narrow grey intervals) of carbon dioxide (A-C), soluble nitrogen (D-F), ammonium (G-I), and nitrate (J-L) dynamics over time, for the three different soil types used in the experiments (column titles; cf. Gras et al., 2010; 2011). Compounds are either represented by their C or by their N content (cf. y-axis labels, Supplement A.1.2).



3. Applications and perspectives

The presented model INDISIM-SOM-NL is accessible to a wide range of potential users, including also soil scientists and students without specific education in programming. It allows exploring the short term SOM dynamics in small scale soil systems corresponding to controlled laboratory experiments with samples incubated at field capacity. Different initial conditions may reflect different soil compositions (e.g. in terms of C to N ratio) or certain amendments (e.g. Supplement A.2). The model also facilitates studying the involved mechanisms and their interactions. For instance, monitoring the usage of different pathways during microbial maintenance and growth reveals *when*, and monitoring the spatial distributions of microbes and relevant compounds reveals *where which* compound is potentially limiting the microbial metabolism (e.g. Supplement A.2). Another example is monitoring the soil's soluble N dynamics (e.g. Fig. 3) to reveal the net effects of interactions of processes that decrease soluble N (microbial maintenance, microbial death) and processes that increase soluble N (microbial metabolism, hydrolysis, cf. Supplement A.1.7).

The model's structure is comprehensible due to the intuitive bottom-up approach of IBMs, defining specific processes for microbial (super-)individuals and for the abiotic environment, and letting the system dynamics emerge from the interactions of these processes. Moreover, users may directly integrate their own ideas of certain microbial behaviors (or additional metabolic groups of microbes, cf. Section 2), abiotic processes, initial or environmental conditions by modifying the model's source code. The required programming knowledge and efforts are considerably reduced owing to the implementation in NetLogo with a clear structure, numerous comments and the full standardized model description (ODD, Supplement A.1). Due to the two-dimensional representation of the soil system, vertical microbial movement and abiotic differences are modeled implicitly (cf. Supplement A.1.2). Transforming the model to an explicit three-dimensional representation is possible (using NetLogo 3D) and would allow considering also vertical gradients and water

flow. Hence, the new model version provides the basis for extensions (e.g. spatially or temporally heterogeneous environmental conditions; cf. Young and Crawford, 2004), and for being coupled to different models (e.g. pore scale models; Gharasoo et al., 2012).

Another important perspective is the integration of novel experimental observations into INDISIM-SOM-NL. The model's emergent dynamics at system level have so far been confronted to conventional soil measurements that determine mass or volume averages (cf. above). Future studies may incorporate also micro scale observations (Baveye et al., 2011), which have become possible through a variety of novel analytical techniques (e.g. Brehm-Stecher and Johnson, 2004; Müller and Nebe-von-Caron, 2010; Watrous and Dorrestein, 2011). Such observational data can be beneficial as direct input (providing parameter values or initial conditions), but also for inverse modeling (being compared to emergent model output to derive parameter values or process definitions). For instance, INDISIM-SOM-NL allows tracking the biomass development and movement of any single SI, observations that may be confronted with experimental data. Following the concept of pattern-oriented modeling (Grimm et al., 2005; Grimm and Railsback, 2012), this facilitates the integration of data at a variety of different scales and hierarchical levels from the whole system to the individuals (Kreft et al., 2013).

4. Conclusions

In comparison to earlier published studies (Ginovart et al., 2005; Gras and Ginovart, 2006; Gras et al., 2010; 2011), the presented new NetLogo version adds to the capacity of the individual-based soil organic matter model INDISIM-SOM in several ways. The simulation model was simplified and unified, and is therefore less dependent on specific assumptions and initial conditions. Various additional means of observation reveal the simulated spatiotemporal dynamics at different scales and hierarchical levels, thus enabling sound analyses of different initial conditions, processes and resulting interactions. The standardized documentation protocol increases the comprehensibility and completeness of the model description, and the implementation in NetLogo makes the model easily accessible to other microbial modelers, for didactical purposes as well as for modifications and extensions. We hope that these advantages will foster the application of INDISIM-SOM and help improving the highly relevant knowledge of how SOM dynamics depend on biotic and abiotic environmental factors (Schmidt et al., 2011), and of soil processes in general (Baveye et al., 2011).

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Appendix A. Supplementary data

Standardized model description, example study of fertilization effects, and sensitivity analysis for time step length and super-individual size (INDISIM-SOM-NL__Supplement.pdf).

Appendix B. Model files

Model software (INDISIM-SOM-NL.nlogo) and initialization files (InitData_Calaf.txt, InitData_Miralles.txt, InitData_Caldes.txt).

Abbreviations

C carbon

N nitrogen

SI super-individual(s)

Figure 1

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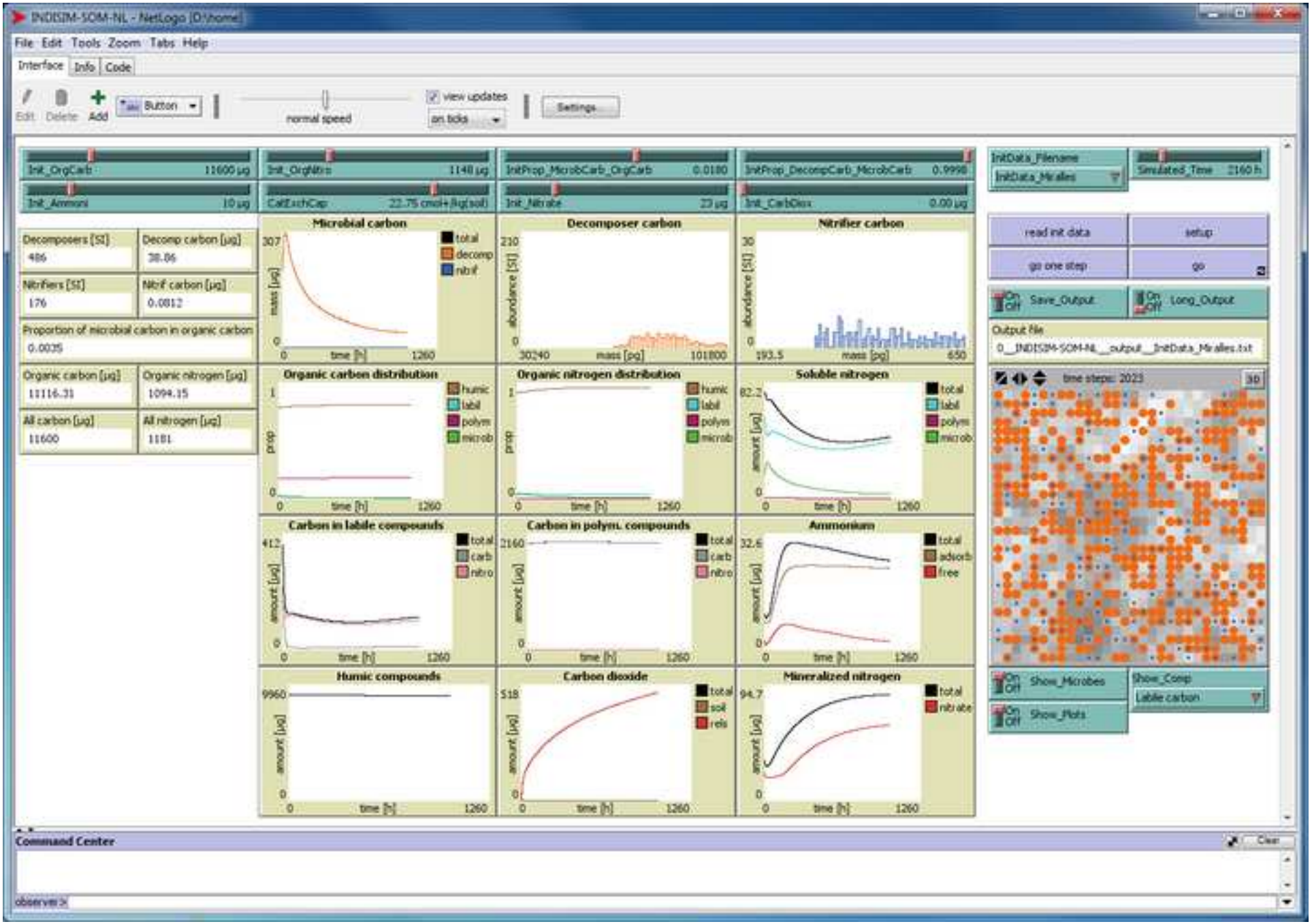

Figure 1 (black&white)

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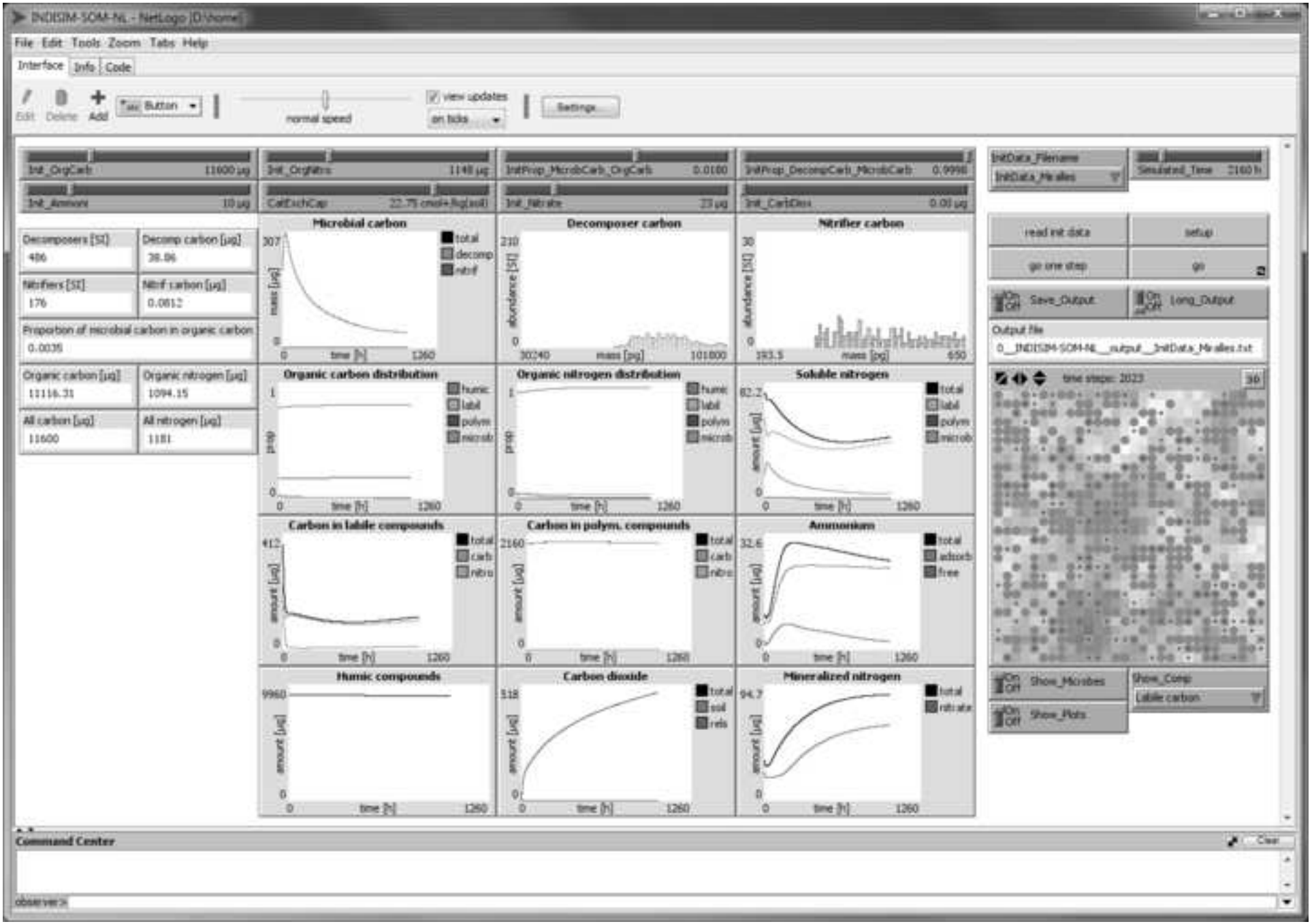


Figure 2

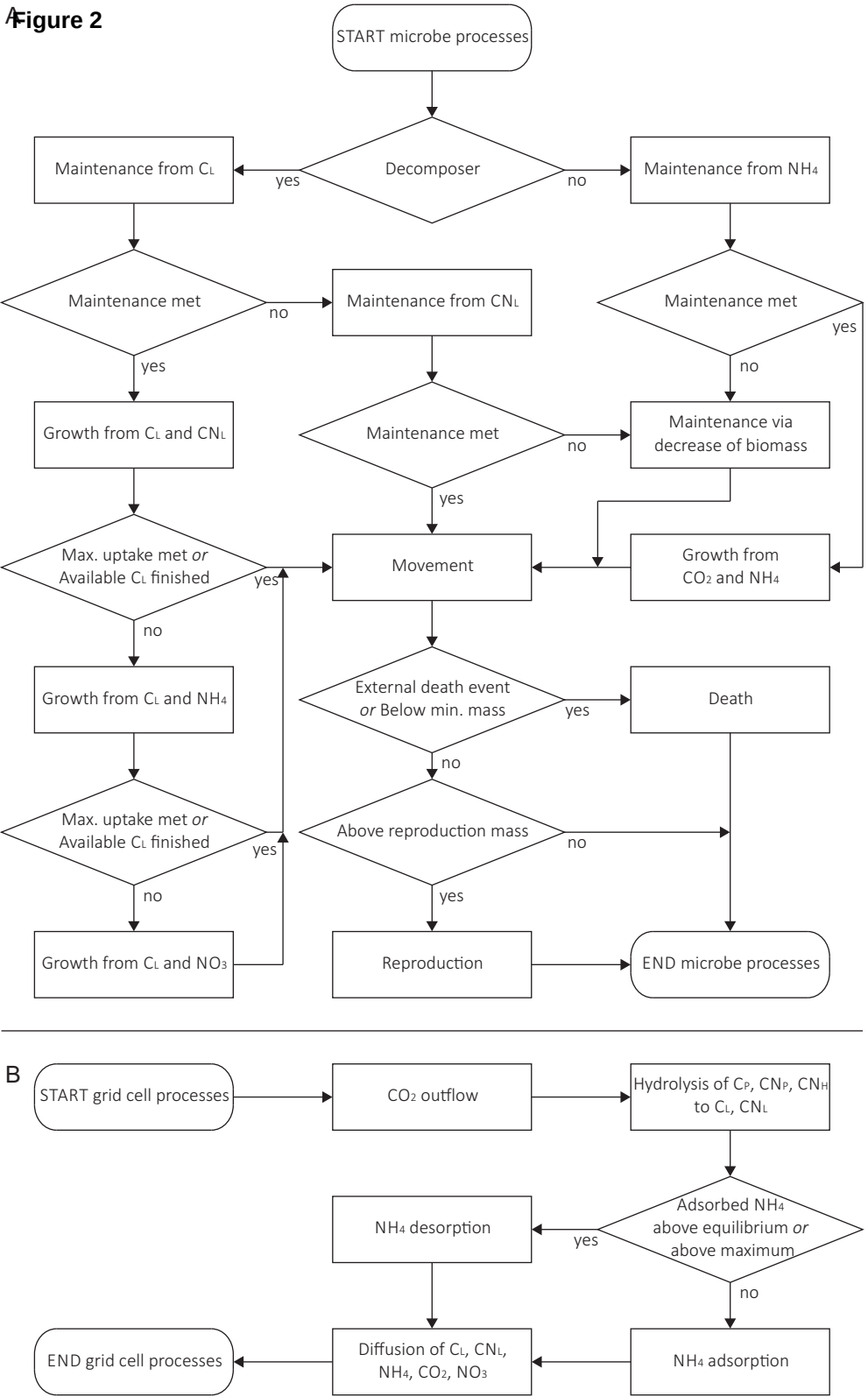
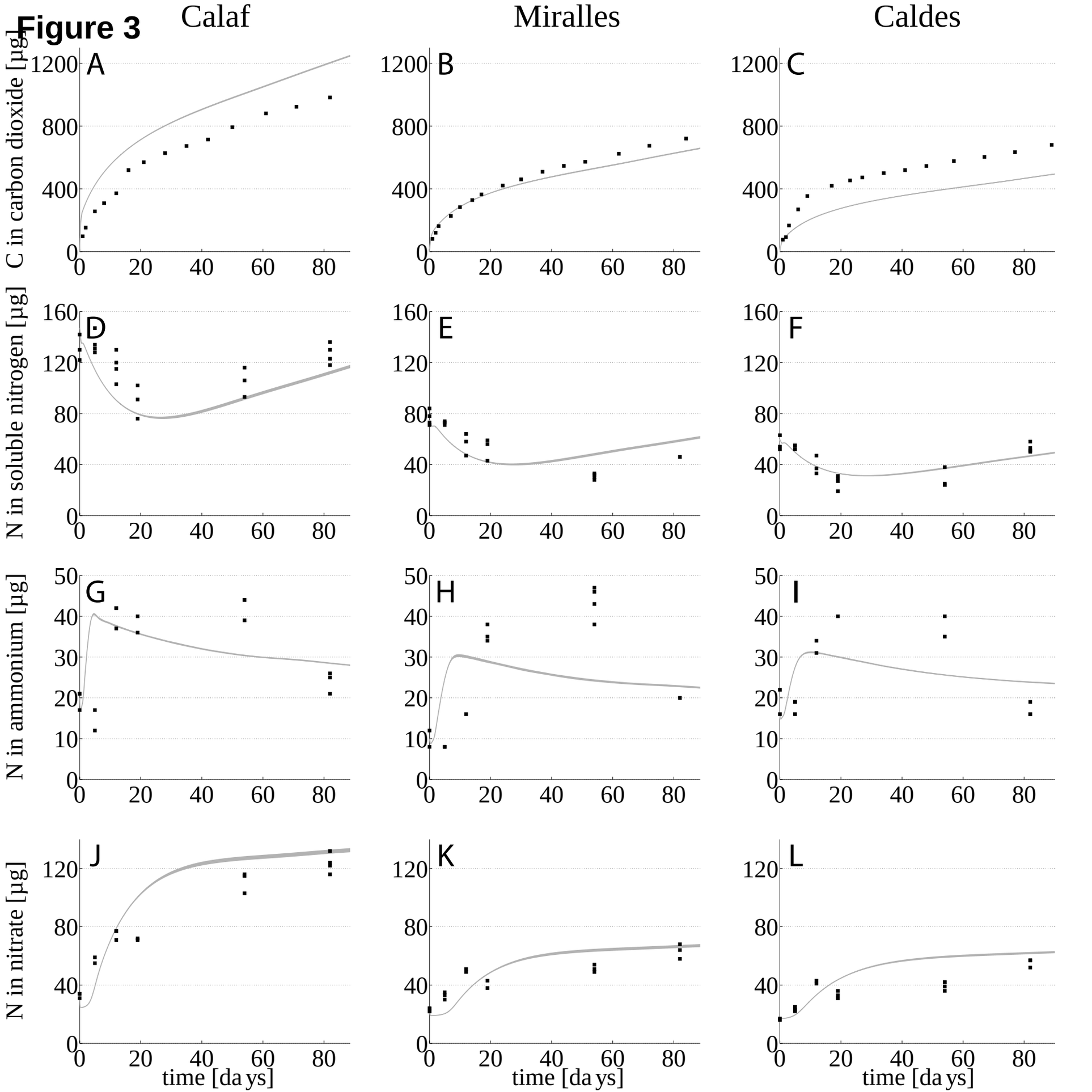

A
START microbe processes
Decomposer
yes
no
Maintenance from C_L
Maintenance from NH_4
Maintenance met
no
Maintenance from CN_L
Maintenance met
yes
yes
no
Growth from C_L and CN_L
Maintenance met
no
Maintenance via decrease of biomass
yes
Max. uptake met *or* Available C_L finished
yes
Movement
Growth from CO_2 and NH_4
no
Growth from C_L and NH_4
External death event *or* Below min. mass
yes
Death
no
Max. uptake met *or* Available C_L finished
yes
Above reproduction mass
no
no
yes
Growth from C_L and NO_3
Reproduction
END microbe processes
B
START grid cell processes
CO_2 outflow
Hydrolysis of C_P, CN_P, CN_H to C_L, CN_L
Adsorbed NH_4 above equilibrium *or* above maximum
yes
NH_4 desorption
no
END grid cell processes
Diffusion of C_L, CN_L, NH_4, CO_2, NO_3
NH_4 adsorption

Figure 3


Calaf
Miralles
Caldes
C in carbon dioxide [µg]
N in soluble nitrogen [µg]
N in ammonium [µg]
N in nitrate [µg]
A
B
C
D
E
F
G
H
I
J
K
L
time [days]
time [days]
time [days]