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Short communication

A new method to determine soil organic carbon equilibrium

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ABSTRACT

This work addresses the dynamical behaviour of the Pasture Simulation Model (PaSim), with respect to the equilibrium conditions for the five carbon (C) pools (structural, metabolic, active, slow, and passive) of soil organic matter (SOM) decomposition, which are modelled according to CENTURY. A novel algebraic approach, based on a sequence of matrices and formulated using the Gauss-Jordan (G-J) elimination algorithm (stable and efficient in memory usage), was proposed and compared to a native iterative procedure using soil C data from 13 European grassland sites. The advantage of the algebraic approach over the iterative method is an enhanced accuracy of C allocation to soil pools and a faster convergence (6–20 times). Its value was discussed in the context of SOM research and modelling.

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Software availability

Name of Software: PaSim (new soil module) Developer: Romain Lardy Contact Address: INRA, UREP, Clermont-Ferrand, France Telephone: +33 4 73624572 Fax: +33 4 73624457 Email: romain.lardy@clermont.inra.fr Availability: on request to the authors Cost: free for no-profit use and team collaboration Program language: Fortran

1. Introduction

Complex models incorporating a mechanistic view of the processes and encompassing the system interactions in a systematic way provide a sound basis for development of generalised response signals of carbon (C) pools, that an analysis of empirical data or a meta-analysis from the literature do not (Guo and Gifford, 2002). In the effort undertaken in the area of soil C modelling, the models developed use the concept of multiple C pools to interpret C dynamics while representing the dynamics of a given system, simulating field responses with a minimal parameter set, and generating signal responses for use in scenario analysis (Hill, 2003). In general, plant material is modelled to enter the soil environment as readily decomposable (sugars and carbohydrates) and resistant (lignin and cellulose) material. The soil components consist of different pools with an associated loss of CO₂ as result of microbial respiration. For modelling the turnover of soil organic matter (SOM), the relative proportion of carbon and nitrogen (C:N) in the plant residue has become the primary mode to divide falling litter into SOM pools of various residence times, varying from months for labile products of microbial decomposition to thousand years for organic substances with firm organic-mineral bonds (e.g. Yadav and Malanson, 2007). Despite the huge diversity in the understanding and interpretation of SOM processes in current models (Falloon and Smith, 2010), the choice of five C pools is generally accepted as appropriate to simulate both C and N in each pool. RothC (Coleman et al., 1997), SOMA (Sohi, 2001) and SOCRATES (Grace et al., 2006) models, for instance, comprise five discrete pools (including inert, slow humic and biomass soil pools) linked by first-order equations, and have been extensively used to understand C turnover from the microbial perspective. CENTURY (Parton et al., 1988) represents soil organic C (SOC) in three conceptual pools (active, slow and passive) with different potential decomposition rates, while above and belowground plant residues and organic excreta are partitioned into structural and metabolic pools.

One potential advantage of these models is that they capture temporal responses, which are important in terms of examining prospective scenarios for climate and anthropogenic modifications

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of the C stock. They generally provide a satisfactory representation of the pattern of C decline under continuous cultivation (Ranatunga et al., 2001). A potential drawback is that in the absence of detailed parameterisation and laborious development of equilibrium conditions for each system, the model behaviour may be unstable or unreliable. Experiments with such models commonly require a steady-state solution for all state variables as a control case or initial conditions (e.g. Chen et al., 2000). Initial equilibrium conditions of the environment (C pools from a starting state, land use and management practices) are often unknown and final equilibrium unreached (Hill, 2003). Pool allocations may have to be arbitrarily assigned, e.g. with pool structures varying in the proportions of C allocated (Hill, 2003). When some information is available on the initial distribution of SOM, the model can be calibrated, e.g. versus soil respiration measurements (Yeluripati et al., 2009).

The most common approach to initialization is to perform long model simulations (e.g. millennia, Wutzler and Reichstein, 2007) to bring the C and N pools to steady state. The process by which a steady-state solution is estimated is referred to as the "spin-up problem" (e.g. Reynolds et al., 2007). In this case, an iterative process may be needed to allocate starting C pool sizes (Ranatunga et al., 2001) that may represent a substantial processing overhead if a large number of simulations must be performed (as with highresolution gridded model applications or for ensemble simulations). However, if soils are apart from equilibrium, spin-up runs may not be always valid (Wutzler and Reichstein, 2007). Moreover, examples are rare of studies that focus specifically on the system dynamics controlling the steady-state solution (Thornton and Rosenbloom, 2005; Martin et al., 2007).

Here we document the dynamical behaviour, with respect to its steady-state solution for the C pools, of SOM decomposition of a particular grassland ecosystem model, the Pasture Simulation Model (PaSim, https://www1.clermont.inra.fr/urep/modeles/pasim.htm) originally developed by Riedo et al. (1998) and based on CENTURY's soil decomposition sub-model (http://www.nrel. colostate.edu/projects/century). The primary purpose of this study was to produce a new spin-up algorithm (matrix-oriented approach) by identifying dynamical constraints (e.g. soil moisture and temperature, nitrogen and carbon soil inputs) that determine the effectiveness of the solution. This was done with the expectation of also improving the simulation quality while reducing the computational cost. In Section 2, the matrix-oriented mathematical

model is provided. An example is considered in Section 3 to illustrate the performance and effectiveness of the approach. Conclusions are drawn in Section 4, where the issue of steady-state solutions is discussed in the context of SOM experimental research and modelling applications.

2. Methods

PaSim is a process-based, grassland biogeochemical model derived from the Hurley Pasture Model (Thornley, 1998) for the plant module, and coupled to CENTURY (version 2) model for the soil processes. PaSim simulates fluxes of carbon, nitrogen, water and energy at the soil-plant-animal-atmosphere interface for managed grasslands (mixed swards) at the plot scale. Weather inputs are on hourly step but grassland processes are simulated on a time step of 1/50th of a day in order to have detailed sub-daily dynamics and assure energy budgets stability. In the soil module structure of PaSim, litter in decomposition over the total soil depth splits into its structural and substrate components, respectively supplying the structural and metabolic soil pools. Other three compartments with different decomposition rates of C between the pools. The kinetics for N flow is essentially similar (chart not shown).

The iterative method originally implemented in PaSim to initialize SOM pools with equilibrium for given climate conditions and management practices (forcing data) proved quite long in execution time (~250 cycles of climatic and management years), with an estimated error (stop criterion for iterations) of ~0.1% of the relative variation in the C balance between two cycles. To overcome such drawbacks, a numerical algorithm was formulated in general algebraic terms using the Gauss-Jordan (G-J) elimination algorithm with full pivoting as inversion algorithm to solve analytically a system of linear equations (adapted from Press et al., 1992). The G-J algorithm was chosen because it is numerically stable and efficient in number of computations and memory usage (e.g. Golub and van Loan, 1996).

The analytical solution relies on annual weather and management cycles. The rationale behind is to use at the end of any given year (or cycle of years) all the information (soil temperature, soil moisture, C and N input fluxes, etc.) of the same year (or cycle of years) to determine the theoretical equilibrium. This process has to be repeated until convergence is achieved, due to the need to maintain equilibrium between the vegetation and the soil. In a matrix-based formulation of the SOM model, the system is represented by a vector $\mathbf{C} = [C_1, C_2, C_3, C_4, C_5]$, where each element C corresponds to C amount in one of the five pools represented in Fig. 1. Eq. (1) represents the variation in the model time step (*dt*), *t* being the instant of simulation:

$$\mathbf{C}'(t) = \frac{\mathbf{C}_{t+1} - \mathbf{C}_t}{dt} \tag{1}$$

This can also be defined as Eq. (2):

$$\mathbf{C}'(t) = \rho_t \cdot \mathbf{A}_t \cdot \mathbf{C}_t + \mathbf{B}_t \tag{2}$$

where $\rho_t = \rho_{T(t)} \cdot \rho_{\theta(t)}$ represents independent temperature, $\rho_{T(t)}$, and water, $\rho_{\theta(t)}$, stress effects; \mathbf{A}_t is the matrix of SOC decomposition rates; \mathbf{B}_t is the vector of C inputs from litter and exudation. The two previous equations can be developed as follows:



Fig. 1. Flow chart of carbon (C) exchanged between the five pools of the PaSim soil module of soil organic matter decomposition.

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