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AggModel: A soil organic matter model with measurable pools for use in incubation studies

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ABSTRACT

Current soil organic matter (SOM) models are empirical in nature by employing few conceptual SOM pools that have a specific turnover time, but that are not measurable and have no direct relationship with soil structural properties. Most soil particles are held together in aggregates and the number, size and stability of these aggregates significantly affect the size and amount of organic matter contained in these aggregates, and its susceptibility to decomposition. While it has been shown that soil aggregates and their dynamics can be measured directly in the laboratory and in the field, the impact of soil aggregate dynamics on SOM decomposition has not been explicitly incorporated in ecosystem models. Here, we present AggModel, a conceptual and simulation model that integrates soil aggregate and SOM dynamics. In AggModel, we consider unaggregated and microaggregated soil that can exist within or external to macroaggregated soil. Each of the four aggregate size classes contains particulate organic matter and mineral-associated organic matter fractions. We used published data from laboratory incubations to calibrate and validate the biological and environmental effects on the rate of formation and breakdown of macroaggregates and microaggregates, and the organic matter dynamics within these different aggregate fractions. After calibration, AggModel explained more than 60% of the variation in aggregate masses and over 70% of the variation in aggregate-associated carbon. The model estimated the turnover time of macroaggregates as 31 and 181 days for microaggregates. Sensitivity analysis of AggModel parameterization supported the notion that macroaggregate turnover rate has a strong control over microaggregate masses and, hence, carbon sequestration. In conclusion, AggModel successfully incorporates the explicit representation for the turnover of soil aggregates and their influence on SOM dynamics and can form the basis for new SOM modules within existing ecosystem models.

1. Introduction

Conventional soil organic matter (SOM) models include three or four carbon (C) pools defined by fixed decomposition rates. For example, the EPIC, CENTURY and DAYCENT models use pools referred to as active, slow and passive with maximum default decomposition rates of 7.3, 0.2, and 0.0045 year^{-1}, respectively (Izaurralde et al., 2006; Parton et al., 1994). Another widely used model, DNDC, uses a labile and resistant microbial SOM pool, a labile and resistant humified SOM pool, and a very labile, a labile, and a resistant residue pool characterized by decomposition rates similar to the CENTURY model (Li et al., 1992). A third model, ROTH-C, uses similar decomposition rates for SOM pools as CENTURY or DNDC, with the exception of an inert SOM pool, for which a decomposition rate of zero is assumed (Jenkinson, 1990). Models based on conceptual SOM pools have been perfected over the past three decades and are reasonably successful in simulating SOM dynamics over decadal time scales as influenced by organic matter inputs and environmental controls, such as temperature and moisture. Although the names of these pools suggest relationships to existing fractions (e.g. humified SOM, bacterial biomass, passive humus, etc.), there are no direct and satisfactory methods to measure the amount of SOM contained in each of these pools within a soil sample (Six et al., 2002a). At best, a correlation between measurable soil fractions and the size of the conceptual pools predicted by SOM models has been found (Skjemstad et al., 2004; Zimmermann et al., 2007). Active pools show some correlation with microbial

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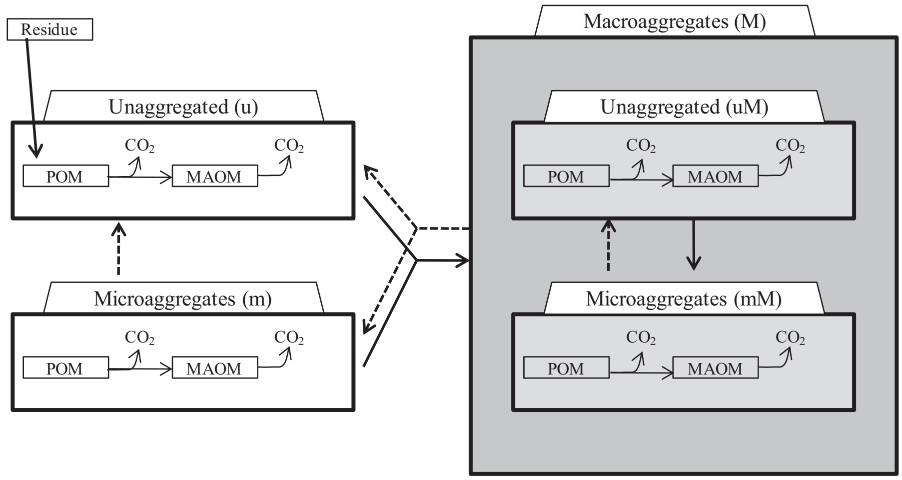

Fig. 1. Conceptual model of soil aggregate dynamics coupled with soil organic matter dynamics. Dashed arrows among aggregates represents aggregate breakdown while solid arrows represent aggregate formation.

biomass and their products, slow pools with resistant plant material and soil-stabilized microbial products (Hsieh, 1992; Metherell et al., 1993), and passive pools with total C (Falloon et al., 1998), black C (Ludwig and Khanna, 2001; Skjemstad et al., 2004), or C-pools resistant to acid hydrolysis (Paul et al., 2001). However, the correspondence often remains very spurious and not generalizable across ecosystems (Six et al., 2002a; Smith et al., 2002). Although these models perform well in predicting decadal datasets of total soil C (Smith et al., 1997), there is a need for models that predict SOM changes in shorter time periods, especially in more detail (e.g. diagnostic SOM fractions; Denef et al., 2007) than total soil C.

We present a conceptual model of soil aggregates dynamics and the role of soil physical structure on the protection of SOM (Fig. 1). Our model is based on the aggregate hierarchy concept (Oades, 1984; Tisdall and Oades, 1982) and divides soil mass into unaggregated (<53 μm) and microaggregated (53–250 μm) soil that can exist within or external to macroaggregated soil (>250 μm) (Cambardella and Elliott, 1993; Six et al., 2004). This hierarchical model creates four unique physical fractions: unaggregated soil external to macroaggregates (u), microaggregates external to macroaggregates (m), microaggregates within macroaggregates (mM) and non-microaggregated soil within macroaggregates (uM) (Fig. 1). Macroaggregates (M, which is the sum of uM and mM) are formed by combining u and m fractions and macroaggregate breakdown transfers soil mass from the M back into the u and m fractions. Microaggregates are predominantly formed within macroaggregates but can breakdown within or external to the macroaggregates (Oades, 1984). Organic matter is largely protected from microbial decomposition once it is enclosed within microaggregates (Angers et al., 1997; Jastrow, 1996; Six et al., 2000) through effects on oxygen diffusion (Sexstone et al., 1985), nutrient accessibility (Golchin et al., 1998) and nutrient adsorption (Linquist et al., 1997; Wang et al., 2001). Since microaggregate formation occurs within macroaggregates, macroaggregate turnover is expected to affect the amount of protected SOM (Six et al., 1998). Understanding the impact of macroaggregate turnover on SOM protection and dynamics is important since its turnover can be manipulated through changes in soil (tillage) management (Denef et al., 2007; Plante and McGill, 2002b; Six et al., 1998).

Previous modeling of aggregate dynamics did not connect aggregate dynamics to SOM dynamics and assumed a constant formation and breakdown of macroaggregates at equilibrium (De Gryze et al., 2005, 2006b; Plante et al., 2002; Plante and McGill, 2002b). However, suppression of microbial activity reduces macroaggregate formation (Bossuyt et al., 2001). Therefore it has been suggested that microbial activity controls the formation rate of macroaggregates (Degens, 1997; Oades, 1984) and that the formation of aggregates is linearly related to the amount of easily decomposable organic matter added (De Gryze et al., 2005). Furthermore, macroaggregate formation is greatest about four days after the peak in microbial respiration, following the addition of fresh organic matter to a soil (De Gryze et al., 2005; Jacobs et al., 2011). Finally, it has been suggested that macroaggregate formation is controlled by two mechanisms: (1) microbial decomposition of plant residues and the resulting production of glue-like or water-repelling binding agents from growing microbial populations (Degens, 1997; Six et al., 2002b) and (2) the proliferation of fungal-hyphae networks (De Gryze et al., 2005; Degens, 1997; Six et al., 2002b).

Sufficient progress has been made in SOM fractionation techniques (Six et al., 1998; Stewart et al., 2008) to be able to develop and validate a SOM model in which physical SOM fractions are included and in which SOM dynamics are directly impacted by their association with physical SOM fractions. We developed a model that is sufficiently flexible to be able to represent all experimental findings summarized above while still remaining simple enough to enable a rigorous validation based on experimental data. Hence, this manuscript introduces AggModel, a simulation model connecting soil aggregate dynamics with SOM dynamics and describes how AggModel is validated with literature data from laboratory incubations. In its current version, AggModel is a proof-of-concept model and intended to simulate aggregate and aggregate-associated C dynamics under simplified laboratory conditions (i.e. constant temperature, constant moisture contents and in the absence of any physical soil disturbance).

2. Materials and methods

Based on the experimental findings outlined in the introduction, the following structure of AggModel is proposed. At the highest level, AggModel consists of two functionally linked hierarchical models, the aggregate dynamics model and the SOM dynamics model, which are linked to each other through a number of feedback mechanisms (Fig. 1). The MATLAB (Math Works, Inc., Natick, MA, USA) source file is given in an online supplement to this article.

2.1. The aggregate model

2.1.1. General description

The aggregate model assumes that all soil mass is present in one of the four soil fractions (i.e. u, m, uM and mM) and therefore aggregate masses are calculated and presented as proportions (Fig. 1). Macroaggregate formation is simulated by transferring equal proportions of m and u into the mM, and uM pools, respectively. The transfer coefficient for this process is $k_{U\rightarrow M}$. Likewise, macroaggregate breakdown transfers equal proportions of mM and uM and their constituents back to the m and u pools, respectively ($k_{M\rightarrow U}$). Microaggregate formation within macroaggregates occurs when soil mass is transferred from the uM to the mM pool ($k_{uM\rightarrow mM}$). The model assumes that microaggregate formation occurs exclusively within macroaggregates (Golchin et al., 1994; Six et al., 2004). The aggregate dynamics model can thus be described with the following differential equations:

$$\frac{dmM}{dt} = -k_{M\rightarrow U} * mM + k_{U\rightarrow M} * m + k_{uM\rightarrow mM} * uM \qquad (1)$$

$$\frac{duM}{dt} = -k_{M\rightarrow U} * uM + k_{U\rightarrow M} * u - k_{uM\rightarrow mM} * uM \qquad (2)$$

$$\frac{dm}{dt} = +k_{M\rightarrow U} mM - k_{U\rightarrow M} m - k_{m\rightarrow u} m \qquad (3)$$

$$\frac{du}{dt} = +k_{M\rightarrow U} * uM - k_{U\rightarrow M} * u + k_{m\rightarrow u} * m \qquad (4)$$

Since the aggregate masses are calculated as proportions of the whole soil, the following equation holds as a corollary of Eqs. (1) until (4):

$$\frac{dmM}{dt} + \frac{duM}{dt} + \frac{dm}{dt} + \frac{du}{dt} = 0 \qquad (5)$$

2.1.2. Simulation of macroaggregate dynamics

Macroaggregate formation rate ($k_{U\rightarrow M}$) is controlled by decomposition of plant residues and proliferation of fungal-hyphae networks (Six et al., 2004). AggModel assumes that the kinetics of these two mechanisms are similarly related to residue addition rate and can be represented by a general microbial activity factor (De Gryze et al., 2005):

$$k_{U\rightarrow M}(t) = k_{U\rightarrow M,\max} f_{MA}(t) \qquad (6)$$

where $k_{U\rightarrow M,\max}$ is the maximal macroaggregate formation rate, which is a function of the amount of organic matter that was added. $f_{MA}(t)$ represents the microbial activity at time t after organic matter addition (see Section 2.3).

Macroaggregate breakdown rate ($k_{M\rightarrow U}$) was modeled as a uniform process with a constant breakdown rate (De Gryze et al., 2005). This rate, in field situations, is known to be increased by disturbances (e.g. raindrop impact, root growth, tillage, etc.) (Denef et al., 2001; LeBissonnais, 1996; Six et al., 1999). However, the available laboratory incubation experiments lack these disturbance factors and therefore are not considered here.

2.1.3. Simulation of microaggregate dynamics

Microaggregate formation is assumed to follow first-order kinetics so that the rate ($k_{U\rightarrow M,\max}$) is constant. Thus, microaggregate formation is directly dependent on the amount of unaggregated soil (<250 μm) within a macroaggregate and macroaggregate turnover time (Six et al., 2000). Likewise, microaggregate breakdown rate is assumed to be equal within and external to macroaggregates and hence $k_{m\rightarrow u} = k_{mM\rightarrow uM}$.

2.2. The SOM model

Each of the four physical locations considered in the model (i.e. u, m, mM, and uM) contain two organic matter fractions: particulate organic matter (POM) and mineral-associated organic matter (MAOM). The POM fraction is operationally defined as organic matter fragments >53 μm and contains organic matter in various stages of decomposition (Besnard et al., 1996; Cambardella and Elliott, 1992). The MAOM fraction is defined as organic material not easily separated from small mineral particles <53 μm and consisting of more transformed and degraded organic matter (Cambardella and Elliott, 1993). Plant residues enter the soil in particulate form and gradually disintegrate during microbial decomposition. With time, the organic matter will be microbially processed and can become part of the MAOM through adsorption onto mineral surfaces. MAOM also consists of the inert organic matter which has turnover times that exceed the duration of experimental incubations and therefore was left out of the model formulation. For each soil fraction X (u, m, mM, or uM), the kinetics of the organic matter dynamics were first-order and modeled as following:

$$\frac{dPOM_X}{dt} = -k_{POM,X} * POM_X + I(t) \qquad (7)$$

$$\frac{dMAOM_X}{dt} = -k_{MAOM,X} * MAOM_X + \alpha_X k_{POM,X} * POM_X \qquad (8)$$

where POM_X and $MAOM_X$ are the amounts of SOM in the particulate and mineral-associated fractions of location X, with $k_{POM,X}$ and $k_{MAOM,X}$ their respective first-order decay rates and I the amount of fresh litter input into the POM. Note that the only direct input of fresh residue occurs into location u, the unaggregated soil. The α_X is a partitioning coefficient regulating the amount of POM that is transferred to MAOM versus mineralized to CO_2. Upon aggregate formation or breakdown, proportional fractions of the POM and MAOM fractions are transferred between the appropriate aggregate fractions.

Therefore, the production of CO_2 can be described with the following equation:

$$\frac{dCO_2}{dt} = (1-\alpha_u) * k_{POM,\,u} * POM_u + (1-\alpha_m) * k_{POM,\,m} * POM_m + \ldots \qquad (9)$$

$$k_{MAOM,\,u} * MAOM_u + k_{MAOM,\,m} * MAOM_m$$

The organic matter dynamics in the system can be described with the following equation:

$$\frac{dOM}{dt} = I(t) - \frac{dCO_2}{dt} \qquad (10)$$

2.3. Model parameterization

Measuring transfer coefficients (e.g. $k_{U\rightarrow M}$, $k_{M\rightarrow U}$, $k_{mM\rightarrow uM}$, $k_{POM,X}$) directly is challenging since the experimental conditions required to measure the coefficients can also reduce aggregate stability. Therefore, experimental measurements likely underestimate the value of the transfer coefficients (De Gryze et al., 2006b) and, hence we used previously published incubation results to calibrate and validate AggModel.

Since microbial activity predominantly controls macroaggregate formation, we used the time-dependent curve of microbial respiration, a proxy for microbial activity, to set the relative macroaggregate formation rate. Specifically, we used the relationship (i.e. f_{MA}) between microbial activity and time after addition of plant residues that was developed by De Gryze et al. (2006b), namely, microbial activity peaks seven days after organic matter addition and decreases to 10% of the maximal rate about 50 days

Table 1
Overview of significant parameters on microbial activity and macroaggregate dynamics. Relative respiration is in relation to maximal respiration and given in percentage, while the other parameters are in days after residue addition.

Reference	Maximal increase in aggregate mass	Decrease of aggregate mass	Maximal respiration	Relative respiration when aggregate mass decreases
Caesar-TonThat and Cochran (2000)	14–28	28–42	NA	NA
Bossuyt et al. (2001)	8–12	NA	2	NA
Denef et al. (2001)	0–14	44–47	2	20
Blair et al. (2005)	0–10	10–20	0–10	NA
De Gryze et al. (2005)	5–9	NA	3	NA
De Gryze et al. (2006a)	2–4	NA	5–15	NA
De Gryze et al. (2006b)	3–7	NA	1	NA
Abiven et al. (2007)	5–10	17–25	5	10
Abiven et al. (2007)	25–33	33–61	5	12
Annabi et al. (2007)	3–7	14–28	3	15
Annabi et al. (2007)	3–7	14–28	3	15
Helfrich et al. (2008)	0–14	14–28	7	40
Helfrich et al. (2008)	0–14	28–56	9	30
Tang et al. (2011)	0–5	15–20	3	50
Jacobs et al. (2011)	3–8	8–14	4	30
De Gryze (unpublished data)	0–7	NA	4–5	NA

NA, not available.

Table 2
Range of soil characteristics and incubation parameters of the acquired datasets.

Parameter	Range	Parameter in model
Organic C in field (gC 100 g^{-1} soil)	0.67–4.4	No
% Clay	7–59	Yes
% Silt	15–82	Yes
% Sand	5–63	Yes
pH	4.6–8.2	No
Incubation temperature	15–25	No
Duration of incubation (days)	21–231	Yes
Residue type	Oilseed rape Wheat corn	No
C:N ratio	10–261	
Soil classification	Orthic luvisol Gleyic luvisols Haplic luvisols Pachic Haplustoll Typic paleudalf Latosol-oxisol	No

after organic matter addition. This is in agreement with other incubation studies (Table 1).

The boundaries of the parameters range were set using findings from published literature and expert opinions (De Gryze et al., 2006b; Plante and McGill, 2002a; J. Six, personal communication, 2011). We acquired data from eight published articles and one unpublished dataset that included 34 different incubation experiments that were relevant to our model (Coppens et al., 2006; De Gryze, unpublished data; De Gryze et al., 2005, 2006b; Denef et al., 2002; Guggenberger et al., 1999; Helfrich et al., 2008; Jacobs et al., 2011). These studies had a large range of soil characteristics and were very diverse in their incubation parameters (Table 2).

We randomly selected half of the dataset to calibrate the different model parameters and the other half to validate our model. A global sensitivity analysis was employed with Monte-Carlo simulations in order to allow the different parameters to vary simultaneously (Saltelli, 2004). We first calibrated the parameters of the aggregate dynamics and then the SOM parameters. Each calibration was performed in two stages. In the first stage, a uniform distribution of each parameter range was established and the model was run on all of the combinations. We used the average un-biased deviation of the simulated calibration data from the measured data to eliminate parameter sets that were not suitable. In the second stage, a random distribution in the range of the parameter sets was established and the model was run on all of the combinations.

Model performance was assessed by comparing the mean squared deviation (MSD) between the modeled and measured proportions of aggregate masses and SOM amounts in the validation dataset (Gauch et al., 2003). The MSD was further partitioned into its three components: squared bias (SB), nonunity slope (NU) and lack of correlation (LC). The SB results from modeled and measured means being different, whereas the NU evaluates the deviation between the modeled and measured data attributed to a slope different to unity. The LC represents the total deviation due to random scatter of the data. All three components are addictive.

3. Results and discussion

As with all soil organic C simulation models, AggModel describes the transfer of organic matter among different C pools and the subsequent gradual decomposition within each of these C pools. Unlike traditional SOM models such as CENTURY, ROTH-C, DNDC or EPIC, the C pools used in AggModel are not conceptual, but directly

Table 3
Soil organic matter and aggregate dynamics parameters, their initial range and their calibrated values.

Parameter	Description	Range	Value (day^{-1})	Turnover time (years)
$k_{U\to M}$	Formation rate of macroaggregate	0–0.85	0.030	
$k_{M\to U}$	Breakdown rate of macroaggregate	0–0.1	0.032	0.086
$k_{uM\to mM}$	Formation rate of microaggregate within macroaggregate	0–0.45	0.010	
$k_{mM\to uM}$	Breakdown rate of microaggregate within macroaggregate	0–0.06	0.006	0.496
$k_{u\to m}$	Formation rate of microaggregate in unaggregated soil	0	0	
$k_{m\to u}$	Breakdown rate of microaggregate in unaggregated soil	0–0.6	0.006	0.496
$k_{POM,m}$	First-order decay rate of POM in microaggregate	0.0001–0.01	0.0006	4.267
$k_{MAOM,m}$	First-order decay rate of MAOM in microaggregate	0.0001–0.01	0.000225	12.177
$k_{POM,u}$	First-order decay rate of POM in unaggregated soil	0.0001–0.01	0.00675	0.406
$k_{MAOM,u}$	First-order decay rate of MAOM in unaggregated soil	0.0001–0.01	0.001	2.740

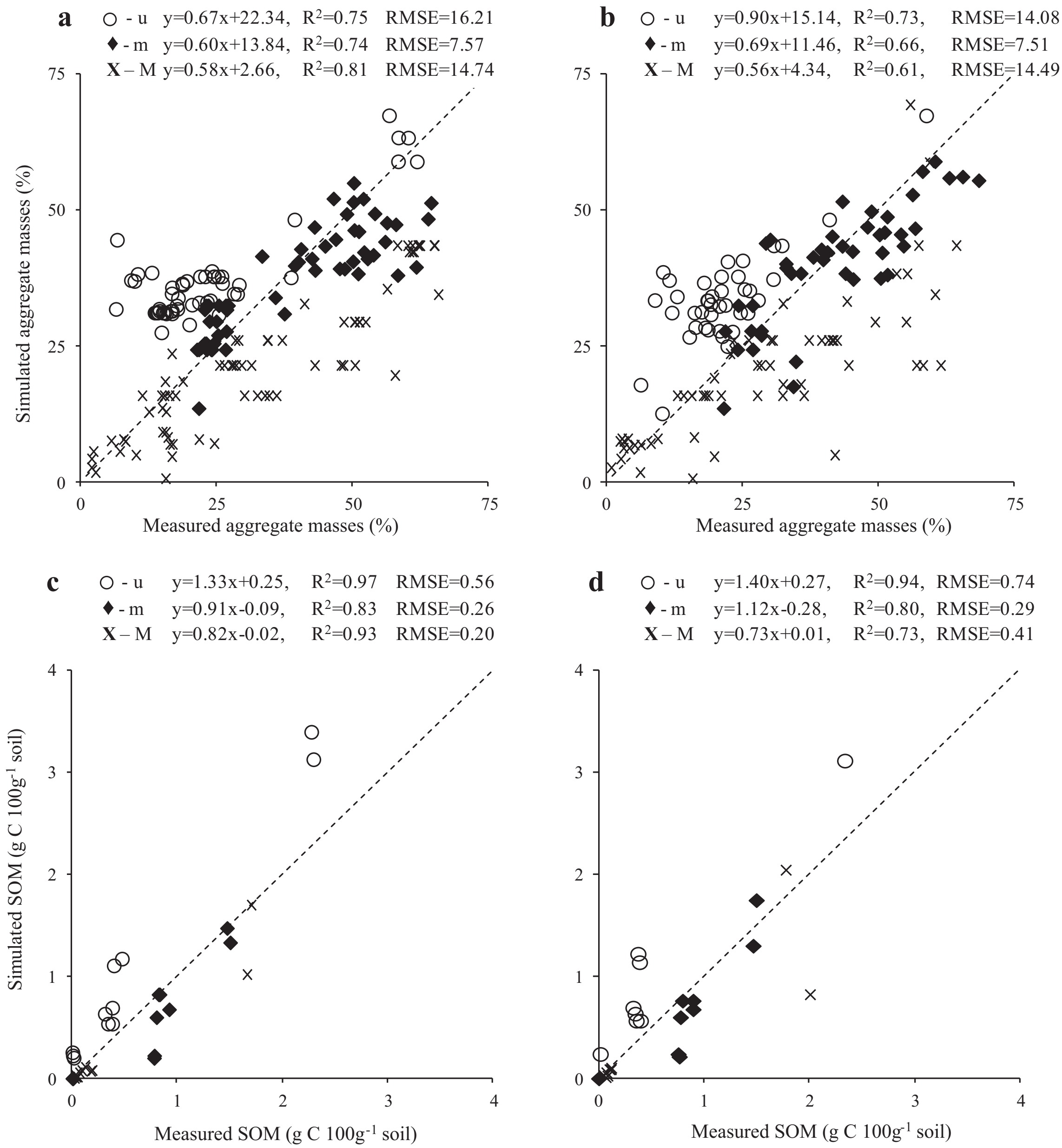

Fig. 2. Relationships between measured and modeled percent of aggregate masses used for calibration (a), percent of aggregate masses used for validation (b), SOM used for calibration (c) and SOM used for validation (d). Dashed line represents 1:1 line.

measurable through physical fractionation techniques (Six et al., 1998; Stewart et al., 2008).

3.1. Model calibration and validation

The calibrated transfer coefficients are given in Table 3 and Table 4. Modeling the validation dataset explained 73, 66 and 61% of the empirically observed variation in unaggregated, microaggregated and macroaggregated masses; respectively (Fig. 2). Furthermore, our model explained 94, 80 and 73% of the empirically observed variation in unaggregated, microaggregated and macroaggregated C contents, respectively.

Most of the MSD can be attributed to LC in the microaggregated masses, macroaggregated masses and in the macroaggregated SOM, which suggest that the prediction error is mostly associated with random scatter of the data (Table 5). Modeled variation for the unaggregated masses and the unaggregated SOM mostly occurred due to SB, however this seems to be acceptable as the coefficient of determination was relatively high compared to the other fractions. The modeled variation of the microaggregated SOM was divided similarly among the three components of the MSD. These correlations were attained by taking into account the amount of residue addition and duration of incubation experiment, while ignoring other important factors (e.g. incubation temperature, soil texture,

Table 4
Soil organic matter partitioning parameters, their initial range and their calibrated values.

Parameter	Description	Range	Value
α_m	Partitioning coefficient of POM between MAOM and CO_2 within microaggregates	0.0001–0.01	0.000225
α_u	Partitioning coefficient of POM between MAOM and CO_2 in unaggregated soil	0.0001–0.01	0.00225

Table 5
Mean squared error (MSD) and its components (SB, squared bias; NU, nonunity slope; LC, lack of correlation) between validated and measured proportion of aggregate masses and SOM.

	Aggregate masses			SOM		
	u	m	M	u	m	M
R^2	0.73	0.66	0.61	0.94	0.80	0.73
MSD	0.020	0.006	0.021	0.549	0.086	0.165
SB (%)	82	5	35	62	36	10
NU (%)	2	0	1	30	25	0
LC (%)	16	95	64	8	39	90

soil mineralogy, quality of residue addition, etc.). The relatively high predictability of the model with the small set of factors included, emphasizes the generality of the model. However, the variance in soil characteristics and incubation parameters that were not included into the model (Table 2) could partly explain the deviation and overestimation of the simulation data from the measured data (Fig. 2 and Table 5).

3.2. Aggregate dynamics

Our model estimated a turnover time of 31 days for macroaggregates (Table 3), which is within the range (9–33 days) of measured turnover times reported in the literature (De Gryze et al., 2006b; Plante and McGill, 2002a). The estimated turnover time of 181 days for microaggregates is larger than the only measured turnover time available in the literature, 88 days (De Gryze et al., 2006b). However, the action of measuring the microaggregate turnover times by rare-earth tracers decreases microaggregate stability, which could lead to an underestimation of the microaggregate turnover time The longer microaggregate turnover time compared to macroaggregate turnover time supports the notion that microaggregates are more stable and therefore protect SOM in the longer term (Edwards and Bremner, 1967; Six et al., 1998; Tisdall and Oades, 1982).

As an example, we present AggModel daily predictions of the mass in aggregate fractions and SOM within aggregate fractions over time following the addition of plant residues at 2 g C 100 g^{-1} soil to an unaggregated soil (Fig. 3). AggModel predicted an initial increase in macroaggregates that peaked about three weeks after plant residue addition and then decreased until the end of the half-year simulation (Fig. 3a). This is consistent with previously published results (Table 1) and supports the hypothesis that macroaggregate formation dominates aggregate dynamics after the initial addition of organic matter, and macroaggregate breakdown dominates when microbial activity decreases to basal levels. Microaggregate formation rate is related to the mass of macroaggregates (Fig. 3a). However, microaggregates (within and external to macroaggregates) peaked about three months after plant residue addition, due to their slower breakdown rate that enables microaggregates to persist for longer periods (Edwards and Bremner, 1967).

The proposed structure of AggModel replicated two important and well-known attributes of a soil system: (1) Macroaggregates dynamics affect microaggregate dynamics; and (2) microaggregates persist in the system for longer periods. These two attributes are central to soil C sequestration in agroecosystems since macroaggregate dynamics can be manipulated through changes in soil management practices, which will eventually affect microaggregates and, therefore, control C sequestration (Six et al., 1998, 2000).

3.3. SOM dynamics

In AggModel, the plant residues enter the u-POM fraction and we observed that within the first month about 50% is transferred into other fractions, with almost 80% into uM-POM (Fig. 3b). About a quarter of the C that is redistributed from uM-POM enters the mM-POM, which transfers more than 80% of its C into the m-POM. These dynamics emphasize the importance of macroaggregate dynamics for the stabilization of C within microaggregates, since although the C in the m-POM originates from the u-POM, it transits through the uM-POM and mM-POM fractions.

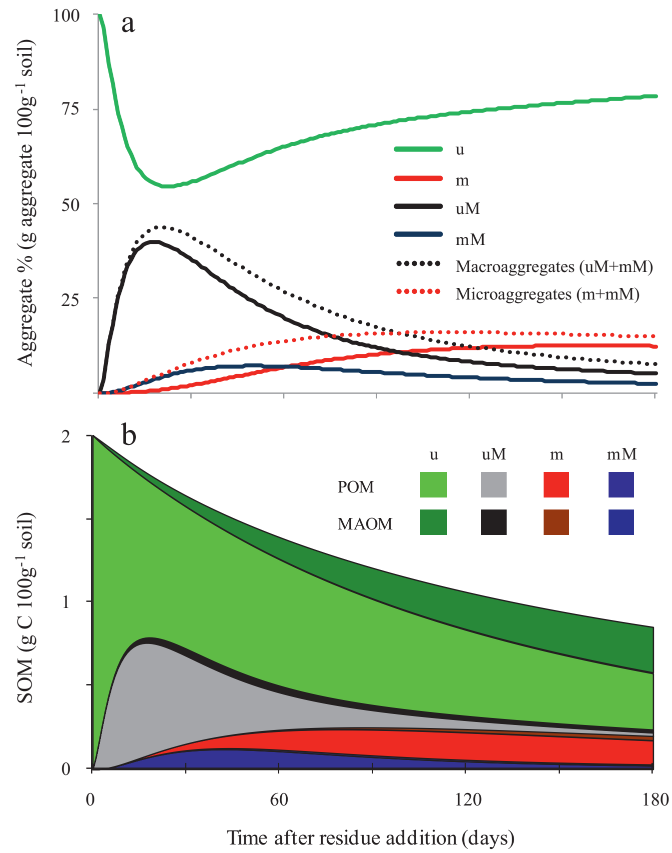

Fig. 3. AggModel daily predictions for (a) soil aggregates and (b) cumulated added SOM within soil aggregates, during half-year simulation after addition of 2 g C 100 g^{-1} soil to an unaggregated soil. u = unaggregated soil external to macroaggregate, m = microaggregates external to macroaggregates, mM = microaggregates within macroaggregates, uM = non-microaggregated soil within macroaggregates, POM = particulate organic matter and MAOM = mineral-associated organic matter.

The total amount of MAOM (i.e. the sum of u-MAOM, uM-MAOM, m-MAOM and mM-MAOM) increases throughout the half-year simulation while the rate of increase reduces within this time-frame (Fig. 3b).

3.4. Robustness of calibrated transfer coefficients

To test the robustness of the calibrated parameter estimates and to understand the relationship among the transfer coefficients and SOM, we ran AggModel varying each transfer coefficient separately, ranging from 50 to 150% of the calibrated values (Fig. 4). Overall, the dynamics of SOM within the aggregates at the end of the half-year simulation are qualitatively similar among the varying transfer coefficients and the calibrated values. This exploration shows that increasing microaggregates (whether directly by increasing microaggregate formation rate, or indirectly by increasing macroaggregate formation rate or decreasing macroaggregate breakdown rate) increases the amount of SOM at the end of the half-year simulation mostly due to an increase in C protected within microaggregates. An opposite trend is apparent when increasing microaggregate or macroaggregate breakdown rate. This

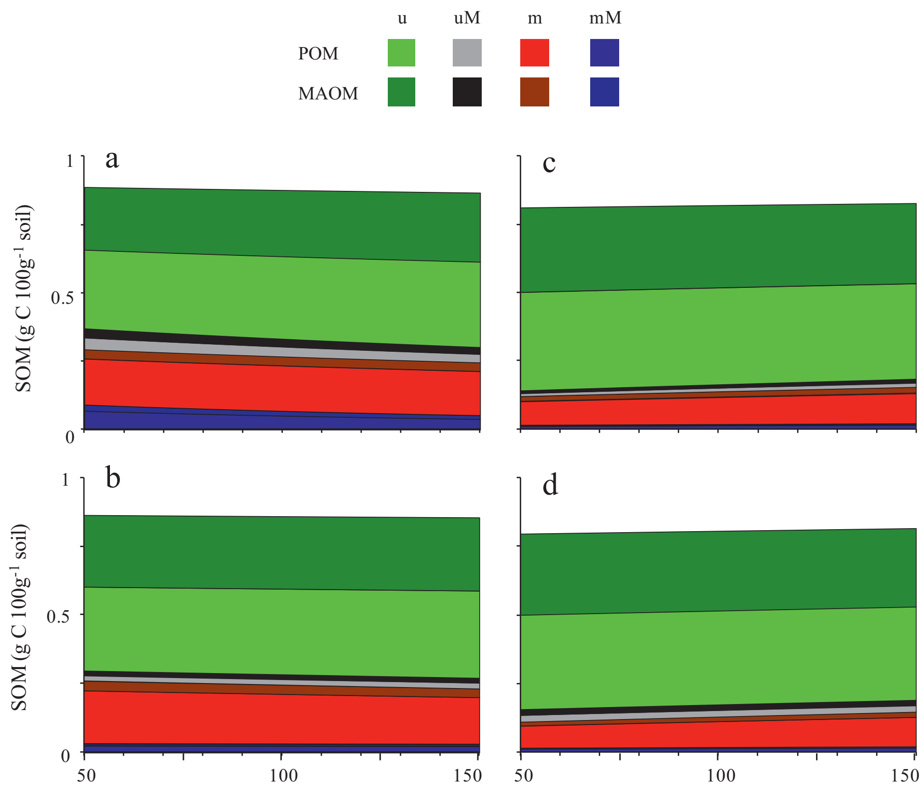

Fig. 4. AggModel prediction of percent carbon at end of half-year simulation as affected by varying between 50 and 150% (a) $k_{M\rightarrow U}$, (b) $k_{m\rightarrow u}$, (c) $k_{U\rightarrow M}$ and (d) $k_{uM\rightarrow mM}$. u = unaggregated soil external to macroaggregate, m = microaggregates external to macroaggregates, mM = microaggregates within macroaggregates, uM = non-microaggregated soil within macroaggregates, POM = particulate organic matter and MAOM = mineral-associated organic matter.

result supports the hypothesis that macroaggregate turnover rate controls C sequestration through its effects on microaggregate formation and survival (Six et al., 1998, 2000).

3.5. *Future model improvements*

Undoubtedly, further development is necessary before AggModel can simulate soils under field conditions. Nevertheless, the potential usefulness of the model is clearly justified through its ability to simulate detailed experimental data and to test hypotheses related to the relationships between SOM and soil structure in a way that no other model has done before.

The current version of AggModel is designed for use under laboratory incubation conditions, in which environmental variables such as temperature and moisture are maintained constant. The following model improvements are required before AggModel can be employed under field conditions:

- Newly formed aggregates are assumed to have the same inherent stability against detrimental forces as older aggregates. However, Denef et al. (2002) showed that frequent dry-wet cycles tended to break up newly formed aggregates but stabilize older aggregates. Assuming a similar stability of all aggregates may not have an effect in incubation settings since all macroaggregates are mostly formed in the first stage following organic matter addition, and therefore the age of formed macroaggregates are similar. Under field conditions, AggModel may need to incorporate more than one single age class of soil aggregates.
- Decomposition of organic matter is assumed to occur as a first-order process without priming effects or other effects of the quality of organic matter added. Future versions of AggModel may need to include priming effects.
- Aggregate dynamics are assumed to be independent of soil texture or mineralogy. Nevertheless, many authors have reported a strong correlation between aggregation and the texture and mineralogy (Denef et al., 2002; Kemper and Koch, 1966). However, texture-dependent differences for aggregates may be primarily related to the texture dependence of raindrop impact or slaking on soil aggregates (Ben-Hur et al., 1998; Six et al., 2004). More research is needed in order to understand the texture-dependent effect on aggregate dynamics before they can be simulated under field conditions.
- For some SOM pools, no satisfactory fractionation technique exists. For example, it is known that a soil contains a substantial amount of passive or inert SOM. Attempts to quantify the size of such a fraction have had limited success (Helfrich et al., 2007). Therefore, the re-introduction of some conceptual pools might be necessary to achieve reasonable model results. However, the main aim of the first version of this model was to describe the dynamics in a medium-term (<1 year) incubation. Since the parameters were optimized based on short-term incubation studies, the parameters related to short time scales could be estimated with much more precision than parameters related to processes that are characterized by longer time scales. Once time series from long-term field experiments (>10 years) are used to validate the model results, we will consider the need for incorporation of a passive pool in AggModel.

4. Conclusions

It has been suggested for over two decades that SOM models should 'model the measurable'. Some recent advances in modeling have been based on measurable fractions, but AggModel, as far as we know, is the first published SOM model that explicitly incorporates the direct and indirect influences of soil aggregation on SOM dynamics. Hence, AggModel is the first step in the development of a SOM model that uses measurable aggregate-associated SOM fractions under field conditions that could be incorporated into existing ecosystem models. Additionally, this proof-of-concept model can also be used for hypothesis generation and testing of hypotheses. For example, the relationship between macroaggregate turnover and microaggregate formation and C sequestration observed in field experiments was successfully simulated by AggModel.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecolmodel.2013.04.010.

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