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Initializing organic matter pools

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Abstract. Organic matter models using multiple pools for soil microbial biomass and soil organic matter have proved able to simulate both short term and long term change in humus content of agricultural soil. However, these pools do not correspond to measurable physical quantities, and are therefore difficult for a non-expert to understand and use. To initialize these pools it is often assumed that organic matter is in a state of equilibrium. Unfortunately, the time to reach equilibrium is often measured in centuries. Therefore the use of a warm-up period cannot replace the need for a good initial partitioning. In this paper we examine a weaker assumption, namely a quasi-equilibrium where all except for the slowest pool is in equilibrium with the amount of carbon input. This assumption allows the non-expert user to initialize the model, and is robust with regard to model changes. We compare the initialization resulting from the equilibrium and the quasi-equilibrium with long term dynamic simulations, and discuss where each method is most applicable.

1 Introduction

Weather-driven simulation modeling has become an important component of studies of soil nutrients and carbon balances in relation to soil quality, environmental impact, and climate change. In relation to carbon balances, organic matter in soil comprises a large storage of terrestrial carbon, which may change with soil use and climate (Levy et al., 2004; Joachim et al., 2007; Riley and Bakkegard, 2006; Foereid and Hogh-Jensen, 2004) affecting the emission of green house gasses, soil quality, and crop production.

In numeric models, it is common to divide the total organic matter (TOM) in the soil into several compartments (Wu and McGechan, 1998; Shaffer et al., 2001), such as recently added organic matter (AOM), soil microbial biomass (SMB), and organic matter that can no longer be traced back to its origin (SOM). These compartments may be further divided into smaller pools, where the content of each pool have uniform properties, such as turnover rate and C/N ratio. In general, having two SOM and two SMB pools allows a well calibrated model to capture both the short term (Jenkinson and Rayner, 1977) and long term (Jenkinson et al., 1987) dynamics of the system. The number of AOM pools depends on the simulating system. For batch experiments and some long time scenarios, a single AOM pool may be enough. However, to simulate input sources from a farming system, a fast and a slow AOM pools per source are in general needed. The dynamics of the modeled system typically consist of input in form of new added organic matter (fertilizer, manure, crop residues) and biologically driven turnover.

A major problem in most organic matter models is to estimate the soil content of the very slowly decomposing or perhaps even inert organic matter pool (Petersen et al., 2005; Bruun and Jensen, 2002). No techniques have facilitated a clear separation of resistant (slow) SOM and easily biogradable (fast) SOM. To initialize these pools it is often assumed that organic matter is in a state of equilibrium (Fontaine and Barot, 2005). Unfortunately, the time to reach equilibrium is often measured in centuries (Wutzler and Reichstein, 2007) and long-term simulations of SOM dynamics are dependent on the initial amount of resistant organic matter. In this paper a weaker assumption is examined, a quasi-equilibrium where all except for the slow, most resistant pool is in equilibrium with the carbon input. Like the equilibrium assumption, the quasi-equilibrium assumption allows the non-expert user to initialize the model, and is robust with regard to model changes.

Before delving into the equations behind the quasi-equilibrium, we will take a look at the Daisy model that will be used for examining it, and the evolution of the model which will provide further context for the initialization problem.

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1.1 Development of the Organic Matter model in Daisy

The organic matter model in Daisy simulates farming practice at field scale, both on the short and the long term. The Daisy code (Hansen et al., 1990, 1991; Abrahamsen and Hansen, 2000) has been validated at several occasions (Shaffer et al., 2001) and has been one of the most accurate in particular with regard to both short and long term predictions of soil organic matter (Vereecken et al., 1991; de Willigen, 1991; Diekkrüger et al., 1995; Smith et al., 1997). Apart from soil organic matter, Daisy also simulates a number of other processes outside the scope of this article, such as water, heat and nitrogen dynamics in the soil, as well as bioclimate, crop development, and management.

The organic matter in Daisy comprises three main compartments: 1) The *added organic matter* (AOM) which for a cultivated soil may include organic fertilizer, crop residuals, including rhizodeposition and dead leaves incorporated to the soil by earthworms. 2) The *soil microbial biomass* (SMB), the living part of the organic matter, excluding roots. 3) Soil humus or *soil organic matter* (SOM), which can no longer be traced back to its origin. The Daisy code allows each compartment to be divided into a user specified number of pools, as well as adjusting the turnover rates, substrate use efficiency (ϵ), the rates of maintenance (for the SMB pools), and directions of flow. Thus, Daisy can be useful as a framework for experimentation with organic matter models.

The original organic matter model in Daisy (Hansen et al., 1990) defined a system with two pools of SOM and SMB, and two pools of AOM for each type of fertilizer applied and crop residues left on the field. It has been modified twice. The first modification was by Müller et al. (1997), and was an adjustment of the turnover rates of the SMB pools so the biomass content of the soil matched the levels measured at the fields. The change did not affect the long time dynamics of the system.

The second change in parametrization was by Bruun et al. (2003). This was a complete recalibration that took into account the carbon input from rhizodepositions. This change was more radical, involving both turnover rates and directions of flow, and made the system much more adaptable to new levels of input. This adaptability has also been directly observed in the field (Heidmann et al., 2001). The recalibration also introduced a new soil organic matter pool, the SOM3 pool, which represents a deactivated, inert SOM pool of humified organic matter. The resulting model, the current standard organic matter model in Daisy, is explained in the next section.

1.2 Organic matter turnover in Daisy

The current standard organic matter model is depicted in Fig. 1.

The amount of carbon turned over and decomposed is directly proportional with the size of the pool. We call this the *turnover rate* by the soil microbial biomass. All the pools in Fig. 1 have a fully drawn outgoing line. From the SOM1 pool the outgoing line is marked with the text “44y”. This indicate the turnover rate of this particular pool and the number is the corresponding halftime (defined as $\ln 2/k$, where k is the turnover rate. For this model, the halftime is 44 years for the SOM1 pool), which means that if there was no input to the pool, the pool would be half the original size after 44 years. For some pools this time is given in days, e.g. the SMB2 pool has a turnover halftime of 69 days.

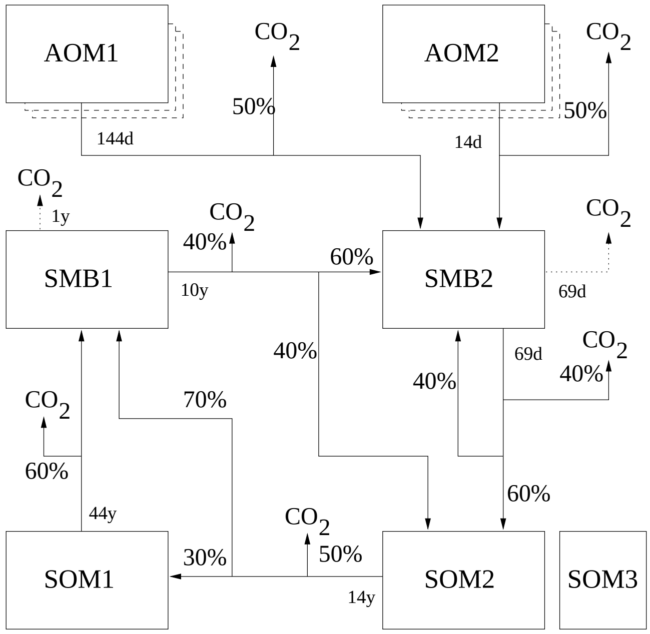

Fig. 1. Current standard organic matter model in Daisy.

If we follow the line from SOM1 it splits into two parts. 60% is completely mineralized and lost as CO_2, the rest is allocated to the microbial biomass in the SMB1 pool. Considering the SOM2 pool, we see that 70% of the carbon not lost as CO_2, are allocated to the microbial biomass and the remaining 30% ends up in SOM1. Besides a turnover rate, the two SMB pools also have a maintenance rate. This rate reflects the cost of staying alive, and is indicated by a stippled line out of the SMB pools. In general, both the rates and the number of AOM pools are variable; the rates given here are just examples. Also, there can be many sets of added organic matter pools, each set corresponds to a particular fertilizer or residual with its specific parameters.

The turnover and maintenance of the pools is affected by abiotic factors, namely the clay content in the soil, the soil temperature, and the moisture. The halftimes listed in Fig. 1 corresponds to 0% clay, 10°C, and field capacity (defined as -100 hPa). The halftimes will increase with increasing clay content, decreasing temperature, and decreasing soil water content, as seen on Fig. 2. Further information of the abiotic factors included in the organic matter model in Daisy is given in Hansen et al. (1990).

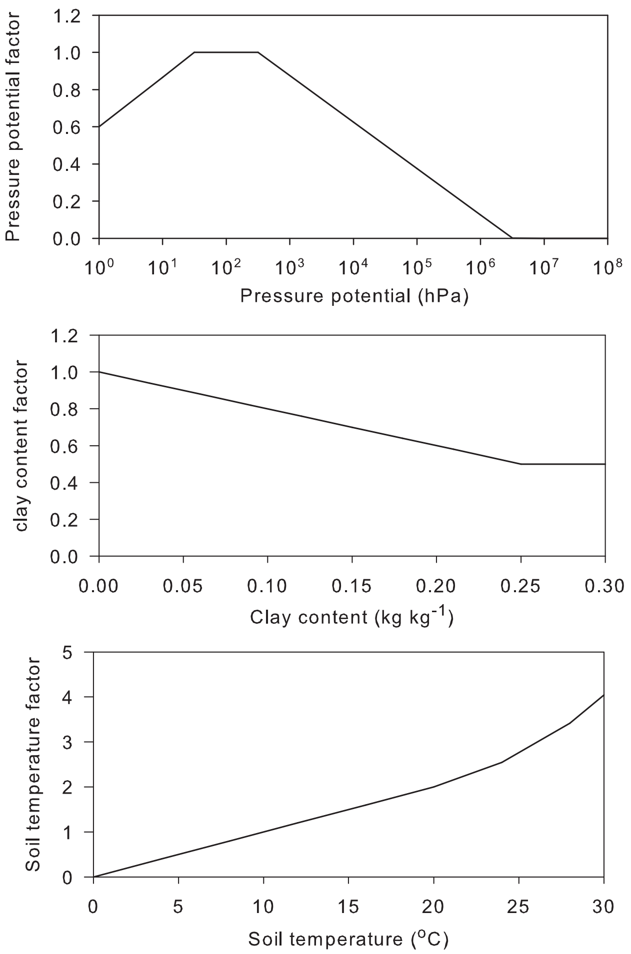

Fig. 2. Effect of abiotic factors on turnover.

2 Initialization of the organic matter pools

Initialization of the partition of the organic matter into the various soil pools have been a particular stumbling block for most users, partly because the partition does not reflect an easily identifiable property of the system being modeled. This lead to the development of a subsystem for initialization of the organic matter pools based on a static approximation of the dynamic model, which will be explored in the next section.

Daisy provides several methods for initialization of the organic matter pools. The largest amount of control can be achieved by explicitly specifying the content of each pool. However, since this requires far more information of both the soil and the model than the user can reasonably be expected to possess, this initialization option is almost exclusively used for hotstarts, that is, restarting the simulation from the saved state of an earlier simulation. Instead, a static approximation of the dynamic organic matter turnover model is used in order to simplify the initialization.

The organic matter model is dynamic due to the uneven application of AOM, and the weather dependent abiotic factors. The static model is achieved by considering average input of added organic matter, and effective static values for the abiotic factors. If we assume the dynamic model is not strongly dependent of the initial conditions, we can combine this initial estimate with a warmup period, to achive a reasonable initial state for the period we are interested in simulating.

For typical use of Daisy (agricultural soil with annual crops) this works well for the initialization of the SMB and AOM pools. After one or two years, the SMB and AOM pools will have adjusted to level of input, and the earlier history will be less relevant. However, as shall be demonstrated in Sect. 3.2, the SOM pools can take centuries to reach equilibrium with new input levels.

2.1 Generalized equations

The rate of change of the individual pools in the dynamic model is governed by Eq. (1).

$$\begin{aligned}
\Delta\text{SMB}i &= \sum_{j=1}^{N_{\text{SOM}}} a_{i,j}\,\text{SMB}j + \sum_{j=1}^{N_{\text{SOM}}} b_{i,j}\,\text{SOM}j \\
&\quad + \textstyle\sum_{j=1}^{N_{\text{AOM}}} c_{i,j}\,\text{AOM}j \qquad ; i = 1 \ldots N_{\text{SMB}} \\
\Delta\text{SOM}i &= \sum_{j=1}^{N_{\text{SMB}}} d_{i,j}\,\text{SMB}j + \sum_{j=1}^{N_{\text{SOM}}} e_{i,j}\,\text{SOM}j \\
&\quad + \textstyle\sum_{j=1}^{N_{\text{AOM}}} f_{i,j}\,\text{AOM}j \qquad ; i = 1 \ldots N_{\text{SOM}} \\
\Delta\text{AOM}i &= g_i\,\text{AOM}i \qquad\qquad\qquad ; i = 1 \ldots N_{\text{AOM}}
\end{aligned} \tag{1}$$

Here, AOMi, SMBi, and SOMi denote the carbon content (mass) of the i'th SMB, SOM, or AOM pool, respectively. ΔAOMi, ΔSMBi, and ΔSOMi denote the change of each pool (mass per time). N_{AOM}, N_{SMB}, and N_{SOM} denote the number of AOM, SMB and SOM pools, respectively.

The relationship between the mass of the pools, and the change of the pools, is assumed to be linear, and denoted by $a_{i,j}$, $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, $e_{i,j}$, $f_{i,j}$ and g_i (fraction per time) respectively. These relationships are calculated on basis of the parametrization of the organic matter turnover model. For example, the formula for finding $a_{1,2}$ can be found in Eq. (2).

$$\begin{aligned}
a_{1,2} = {} & (t_{\text{SMB1}}\,(X_{\text{SMB1}\rightarrow\text{SMB2}}\,E_{\text{SMB1}} - 1) - m_{\text{SMB1}}) \\
& F^{T}_{\text{SMB1}}(T)\,F^{\psi}_{\text{SMB1}}(\psi)\,F^{C}_{\text{SMB1}}(X_c)
\end{aligned} \tag{2}$$

Where t_{SMB1} is the turnover rate and m_{SMB1} is the maintenance of the SMB1 pool. $X_{\text{SMB1}\rightarrow\text{SMB2}}$ is the carbon fraction going from SMB1 to SMB2. E_{SMB1} is the efficiency of which SMB1 can be decomposed, the remaining part is lost to the atmosphere as CO_2. F^{T}_{SMB1}, F^{ψ}_{SMB1}, and F^{C}_{SMB1} are functions describing the effect of the abiotic factors for soil temperature, moisture, and clay, respectively. The other relationships in Eq. (1) can be described by similar forms.

2.2 Known and unknowns

For initialization purposes, we assume that the temperature and soil humidity are constant and known, which means $a_{i,j}$, $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, $e_{i,j}$, $f_{i,j}$ and g_i will also all be known constants. This still leaves us with one equation, and two unknowns (content and change) for each pool in our system. In order to find a solution, we will need further assumptions to either increase the number of equations, or decrease the number of unknowns.

2.3 Initialization methods

The Daisy software provides the user with six methods for initialization, each will result in a linear equation system that can be solved using a standard technique (Gauss-Jordan elimination is used in Daisy). The methods will be listed in the following sections. All the methods rely on the assumption that the SMB pools are in equilibrium, meaning $\Delta\text{SMB}i$ are all zero Eq. (3).

$$\Delta\text{SMB}i = 0 \qquad ; i = 1 \ldots N_{\text{SMB}} \tag{3}$$

This is reasonable as the SMB pools tend to adjust to input levels relatively fast (a few years at most). All but one initialization option require the user to specify the total organic matter in the soil, which allows us to add Eq. (4) to the system without increasing the number of unknowns.

$$\text{TOM} = \sum_{i=1}^{N_{\text{SMB}}} \text{SMB}i + \sum_{i=1}^{N_{\text{SOM}}} \text{SOM}i + \sum_{i=1}^{N_{\text{AOM}}} \text{AOM}i \tag{4}$$

The final common assumption is that the carbon input is known, as in Eq. (5).

$$\Delta\text{AOM}i = k_i \qquad ; i = 1 \ldots N_{\text{AOM}} \tag{5}$$

Here k_i denote the known carbon input to AOMi, from which the size of AOMi can trivially be found given Eq. (1) (AOM$i = k_i/g_i$), and eliminated as unknowns from the equation system.

Combining all three assumptions, we still lack $N_{\text{SOM}} - 1$ equations before we can solve the system.

2.4 Method 1: Explicit SOM partitioning

The original, and still supported, method of initializing the SOM pools was to require the user to explicitly specify the fraction of the total SOM allocated to each pool, at in Eq. (6).

$$\text{SOM}i = f_{\text{SOM}i} \sum_{j=1}^{N_{\text{SOM}}} \text{SOM}j \qquad ; i = 1 \ldots N_{\text{SOM}} \tag{6}$$

where $f_{\text{SOM}i}$ are user supplied fractions. This gives us N_{SOM} additional equations, however since $\sum_{i=1}^{N_{\text{SOM}}} f_{\text{SOM}i} = 1$ the system is overspecified, and we leave out one of the equations. That is, for a system with two SOM pools, we only specify one equation, $\text{SOM}1 = f_{\text{SOM}1}(\text{SOM}1 + \text{SOM}2)$. Thus, Eqs. (6), (3), (4), and (5) this gives us enough equations to find a solution.

The explicit SOM partitioning gives the user good control over the simulation with a manageable number of parameters. However, the SOM partitioning is model specific, and does not correspond to measurable quantities.

2.5 Method 2: Background mineralization

For simulations where our main interest is in the soil organic matter as a nitrogen storage, Daisy allow the user to specify desired background mineralization levels. The background mineralization is defined as the decrease over time of nitrogen stored in the SOM pools. Assuming a constant C/N ratio for each pool (C/N$_{\text{SOM}i}$), gives us the equation

$$background = \sum_{i=1}^{N_{\text{SOM}}} \frac{\Delta\text{SOM}i}{\text{C/N}_{\text{SOM}i}} \tag{7}$$

This gives us one extra equation. In the case of two SOM pools, we then have enough equations to find a solution. Using background mineralization for initializing the system has the advantages of being model independent and even indirectly measurable, but requires a good understanding of the nitrogen dynamics of the system.

2.6 Equilibrium assumptions

If the system is in equilibrium, none of the pools will change, so we can add Eq. (8).

$$\Delta\text{SOM}i = 0 \qquad ; i = 1 \ldots N_{\text{SOM}} \tag{8}$$

Together with Eqs. (3), (4), and (5) this gives us one more equation than needed, so Daisy will allow the user to relax some other assumption. This leads to the three different variants explained in the following.

2.6.1 Method 3: Size of inert pool

If we have an inert pool, like SOM3 in Fig. 1, adding an equation stating that $\Delta\text{SOM}3 = 0$ does not add any additional information (it is already part of Eq. (1), where $d_{3,j}$, $e_{3,j}$, and $f_{3,j}$ will be 0 for all j). This is the case for the default initialization of the subsoil, here we assume the active pools are in equilibrium with the input, and let the equation system find the size of the inert pool.

2.6.2 Method 4: Total organic matter

The second equilibrium initialization allows the user to leave out Eq. (4), so the total amount of (active) soil organic matter is estimated from the input levels. This is rarely useful, as total amount of organic material is easy to measure, but has been used in this paper to initialize the organic matter content for long term simulations in section 3, where we examine the period from one equilibrium to another.

2.6.3 Method 5: Unknown input

The last and most common equilibrium initialization is to let the user specify the size of the inert pool (usually to zero), and leave out Eq. (5). This is useful for cases where the user have no idea of what the input levels for the field used to be.

2.7 Method 6: Quasi-equilibrium

The default initialization for organic matter in the plough layer is to weaken the equilibrium assumption, and allow the pool with the lowest (non-zero) turnover rate to change. That is, we remove one of the equations added by Eq. (8), namely for the slowest active pool, typically SOM1, and keep all of Eqs. (3), (4), and (5). The idea is that all the fast pools will quickly adapt to the input and to the size of the slow pool.

3 Simulations

In this section, we compare the static solutions we get with the equilibrium and the quasi-equilibrium assumptions from the previous section, using a dynamic simulation as a baseline, and the model described in Sect. 1.2 with an empty SOM3 pool. In the dynamic simulations we follow a system that goes from equilibrium at one level of carbon input, to equilibrium at another input level. In particular we follow the relative size of the two active SOM pools.

3.1 Driving variables and soil parameters

Since the organic matter paramterization in Daisy has been developed based on Danish soils, we have used Danish data for all simulations.

3.1.1 Weather

The weather data are from an meteorological research station in Taastrup, in the Eastern part of Denmark. A time series from 1970 to 1999 was used, and was repeated for the entire simulation. The simulation period was 600 years.

3.1.2 Soil

To include the effect of clay content, two standard soils for Danish conditions have been selected, a coarse sand typical for the Western part of Denmark, and a sandy loam typical for the Eastern parts of Denmark. The particle size distribution and dry bulk density ρ_b of the two soils are listed in Table 1. The total organic matter is not listed, as we initialize it to be in equilibrium with the specified input. Only the plow layer (0–30 cm) is considred in the simulations.

Table 1. Particle size distribution and dry bulk density ρ_b of the two standard soils.

Soil	clay (<2 μm)	silt (2-50 μm)	sand (50-2000 μm)	ρ_b g/cm^3
Sand	3.9	6.4	89.7	1.45
Sandy loam	12.4	24.9	62.7	1.53

3.1.3 Management

Two management practice of high and low C-input to the simulated systems have been evaluated for each soil. For the coarse sand also a medium C-input management was included. All the management practices have been taken from Styczen et al. (2005). Table 2 lists the average C-input together with the average and initial abiotic factor and the initial C-input of the different management and soil combinations. The total C input is higher in the sandy loam soil than in the sandy soil because crop production is higher, which results in a higher input of residuals.

Table 2. Average input of organic C to thw plow layer (0–30 cm) and average abiotic factor (heat factor times humidity factor) in simulated management for sandy and sandy loam soils. The initial abiotic factor and initial C refers to the initialization of the organic matter module using equilibrium assumptions. The unit for C input is kg C ha^{-1} y^{-1}. The average abiotic factor was also used for initialization, thus only one number is listed in the table.

Soil	Manag.	average C input	abiotic factor	initial C input	initial TOM
Sand	Low	1817	0.680	5200	?
Sand	Medium	4412	0.680	5200	?
Sand	High	5158	0.681	1800	?
Sandy loam	Low	2283	0.622	6500	?
Sandy loam	High	6525	0.623	2300	?

3.1.4 Abiotic factors

For the initialization we must use constant values. This is not a problem for clay, which varies little within the time frames we are concerned with, but problematic for the temperature and hummidity effects. By default the Daisy model use the local average air temperature (which is already specified by the user in the weather file) for T, and field capacity (-100 hPa) for the water potential. A better estimate can be achieved by logging the product of factors in a realistic simulation.

Figure 3 shows the variation of the product of the heat and humidity effects within a specific year for both the sand, and the sandy loam. The abiotic factors for the two soils are equal during the winther, where the humidity is high enough that only the temperature has an effect. This is typical for Danish conditions. During the summer, the sand gets dryer than the sandy loam, so the combined factor is also lower.

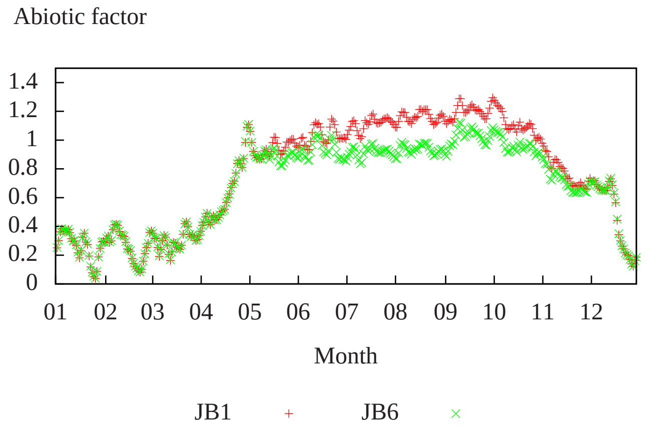

Fig. 3. The combined heat and humidity effect (y-axes) for a sand (+) and sandy loam (×) as it varies over a year (x-axes).

Figure 4 shows the variation between years of the combined heat and hummidity effect over the 30 years of climate used, as well as a running average. As can be seen, at least for Danish conditions, long time series are required before it makes sense to talk about effective values, due to the high variation.

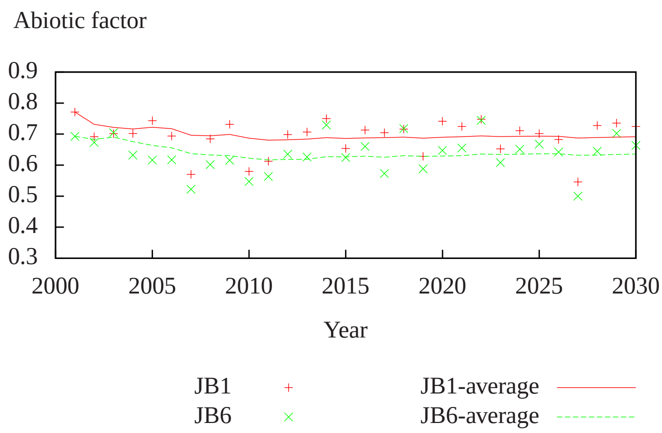

Fig. 4. The combined heat and humidity effect (y-axes) for a sand (+) and sandy loam (×) as it varies between years (x-axes). The stippled lines are the running averages for the two soils.

3.2 Results and discussion

Figure 5 shows the results of switching between low and high carbon input for the two soil types. With the organic matter model described in Sect. 1.2. Full equilibrium always corresponds to 49% SOM1 (Bruun and Jensen, 2002), which is where the SOM1 begins and ends in all four graphs. A more moderate change is depicted in Fig. 6.

After a decrease in input (Fig. 5, top), the organic content of the soil decreases, but the easily degradable SOM pool (SOM2) decreases faster than the more resistant pool (SOM1), so the relative SOM1 fraction increases temporarily. A similar effect can be seen after an increase of input (Fig. 5, bottom), where the easily degradable SOM pool build up faster than the resistant pool, and relative SOM1 fraction decreases temporarily while the total organic matter builds up.

Equilibrium is reached after 200 (sandy loam, increasing input) to 600 (sand, decreasing input) years. Since the longest experimental trial used for validating the organic matter model in Daisy is 70 years (Smith et al., 1997), these results must all be viewed as extrapolation. Equilibrium is reached sooner for the sandy loam than for the sand, and sooner for increasing input than for decreasing input. For decreasing input, quasi-equilibrium is reached after 150 years (on sand) or 100 years (on sandy loam), well before equilibrium. For increasing input, quasi-equilibrium is reached at approximately the same time as equilibrium.

The initialization method developed here is easy to understand and use by the user. The two mandatory numbers are the total content of organic matter, and an estimate of how much carbon has been added to the system per year in the recent decades. The total content of organic matter is directly measurable and the carbon input estimated by the user, for example from the use of Daisy simulations. None of the these numbers need to be changed when the model itself is changed.

As can be seen, the time to reach a new equilibrium after a large change in farming practice can be several centuries, which makes it safe to assume that Danish farming land is not in equilibrium. At such a time scale, not only farming practice but also climate is going to change.

After lowering carbon input, we reach quasi-equilibirum at around a third of the time we use to reach full equilinbrium. For a large change, this unfortunetely is not practically useful, as even for the scenario where the quasi-equilibirum does best (the sandy loam), it still takes a century to reach quasi-equilibirum. In the case of raising carbon input, quasi-equilibirum doesn't seem to be approached faster than full equilinbrium. For relatively small changes in carbon input, either method works fine.

In all scenarios, the quasi-equilibirum estimate for SOM1 approaches the value predicted for full equilibrium (49%, Bruun and Jensen (2002)) as the dynamic model itself approaches equilibrium. Since the quasi-equilibirum estimate is strongly dependent on abiotic factors, this indicates that, despite the non-linearity of the abiotic effect functions, using the average value work well, under the conditions examined. The average value can be found with a Daisy simulation.

Despite the increased clay content, which should slow down turnover in the system, the sandy loam reach both quasi-equilibirum and full equilibrium faster than the sand, because of the increased humidity of the soil during the summer. Which indicate that both initialization assumptions would result in estimates of the SOM partitioning that are closer to the dynamic model, under climate where organic matter turnover is faster due to heat or humidity.

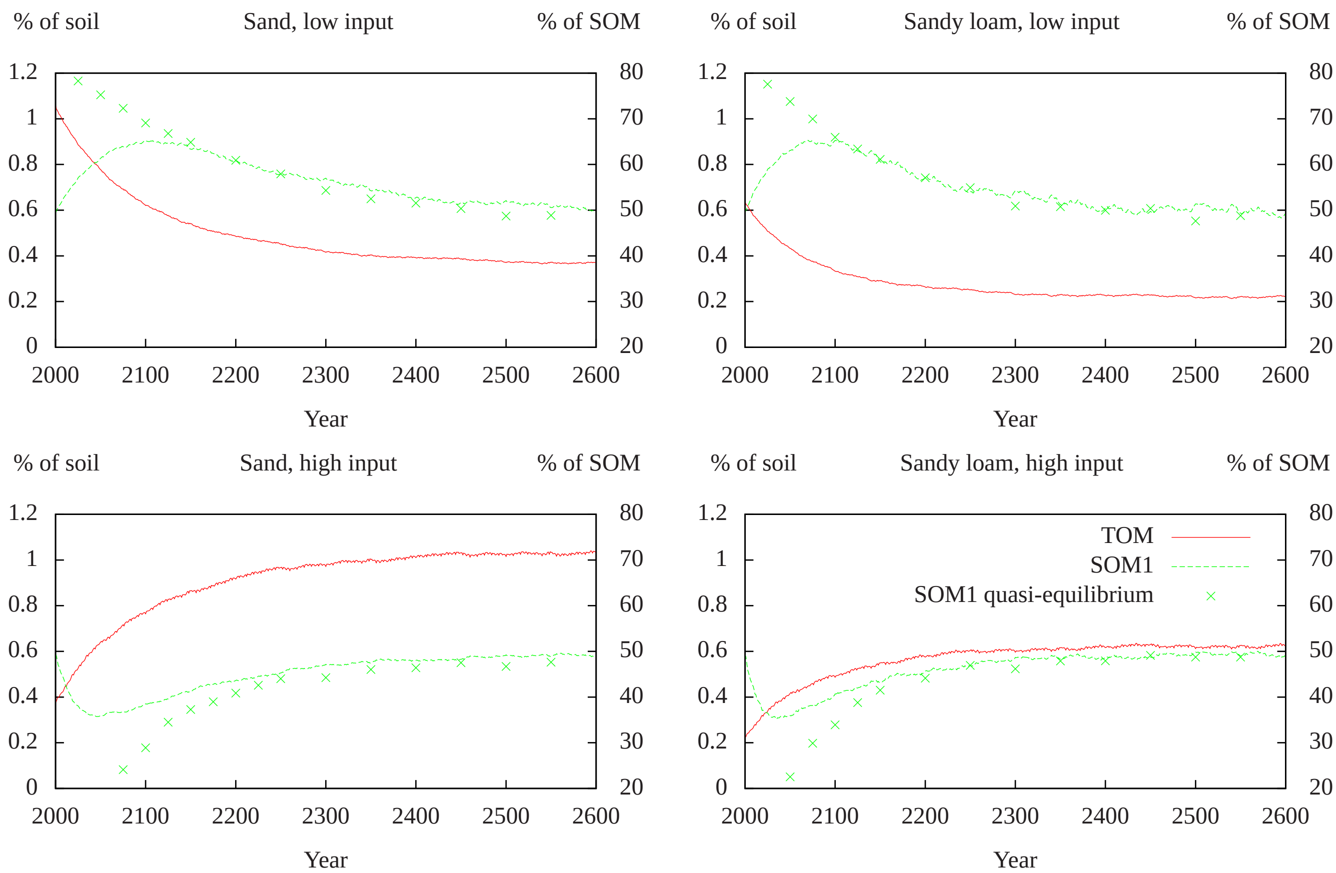

Fig. 5. Long term simulation on a sand (left column) and sandy loam soil (right column) of total organic matter (TOM) in percent of soil dry bulk mass (fully drawn line, left axes) and SOM1 in percent of of total SOM (dotted line, right axes) with management changing from: (top row) high to low C input and (bottom row) low to high C input. The $\times$'s indicate the initialization of SOM1 for the current amount of TOM estimated by the quasi-equilibrium.

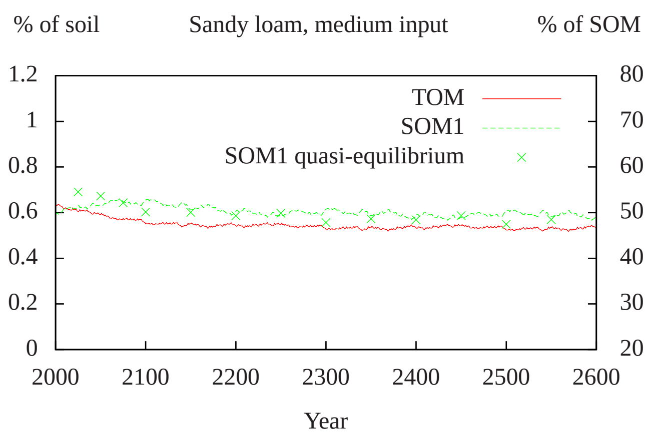

Fig. 6. Long term simulation on a sand of total organic matter (TOM) in percent of dry bulk mass (left axis) and SOM1 in percent of toal SOM (right axis) with management changing from high to medium C input. Simulated values are on the dotted line. The $\times$'s indicate the initialization of SOM1 for the current humus level estimated by the proposed quasi-equilibrium.

Another possible aspect for further study would be other organic matter model parametrizations, especially parametrizations where difference in the turnover rate between the SOM pools is higher.

4 Conclusions

The quasi-equilibirum assumption doesn't work under Danish conditions with the current organic matter model in Daisy.

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