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C-TOOL: A simple model for simulating whole-profile carbon storage in temperate agricultural soils

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ABSTRACT

Soil organic carbon (SOC) is a significant component of the global carbon (C) cycle. Changes in SOC storage affect atmospheric CO_2 concentrations on decadal to centennial timescales. The C-TOOL model was developed to simulate farm- and regional-scale effects of management on medium- to long-term SOC storage in the profile of well-drained agricultural mineral soils. C-TOOL uses three SOC pools for both the topsoil (0–25 cm) and the subsoil (25–100 cm), and applies temperature-dependent first order kinetics to regulate C turnover. C-TOOL also enables the simulation of ^{14}C turnover. The simple model structure facilitates calibration and requires few inputs (mean monthly air temperature, soil clay content, soil C/N ratio and C in organic inputs). The model was parameterised using data from 19 treatments drawn from seven long-term field experiments in the United Kingdom, Sweden and Denmark. It was found that the initial SOC content had to be optimised for each experiment, but also that one set of values for other model parameters could be applied at all sites. With this set of parameters, C-TOOL can be applied more widely to evaluate effects of management options on SOC storage in temperate agricultural soils. C-TOOL simulates observed losses of SOC in soils under intensive agricultural use and the gain in SOC derived from large inputs of animal manure and inclusion of perennial grassland. The model simulates changes in SOC for the entire profile, but lack of data on subsoil SOC storage hampers a proper model evaluation. Experimental verification of management effects on subsoil C storage, subsoil C inputs from roots, and vertical transport of C in the soil profile remains prioritised research areas.

1. Introduction

Soil organic carbon (SOC) in the form of organic matter not only contributes to soil quality, it also accounts for about twice as much as the carbon (C) found as CO_2 in the atmosphere (Lal, 2004). Major uncertainties in the global C budget are associated with changes in SOC stored in agricultural soils (Stockmann et al., 2013). Losses of SOC from previous and current soil management remain an important source of atmospheric CO_2, with SOC stocks continuing to decline for decades to centuries after the start of cultivation (Johnston et al., 2009). A number of abiotic factors exert an overall control of SOC in long-term agricultural soils, but for a given soil within a given climate, changes in SOC storage are determined by land use and management. Since changes in SOC contents occur slowly and against a large background of C already present in the soil, repeated soil sampling over decades is needed to experimentally verify effects of specific changes in land use and soil management (Saby et al., 2008; Smith, 2004). Estimates of overall changes in SOC storage have been based on regional inventories (Capriel, 2013; Chapman et al., 2013; Heikkinen et al., 2013; Meersmans et al., 2009), simulation models (Andrén et al., 2008; Kirk and Bellamy, 2010; van Wesemael et al., 2010; Webb et al., 2003) and on data from long-term field experiments (Kätterer and Andrén, 1999; Powlson et al., 2011; Smith et al., 1997).

Reliable projections of changes in SOC at farm- and regional-scales are required to predict the impact of agricultural activity on the global C cycle, to estimate the responses of climate changes and to allow farmers and policy makers to develop and implement management options that may reduce CO_2 emissions from agricultural soils and protect the soil resource. Dynamic process-oriented simulation models are generally considered to be efficient tools for projecting the effects of management on SOC and several

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models are able to simulate C turnover in agricultural soils. Some are dedicated C models (e.g. RothC, ICBM, and Yasso07 (Andrén and Kätterer, 1997; Coleman and Jenkinson, 1996; Tuomi et al., 2009)), while other models include nitrogen (N) and water, or have a scope that extends to the ecosystem level (e.g. DNDC, CENTURY and Daisy (Hansen et al., 1991; Li, 1996; Parton et al., 1987)). Most contemporary models are heavily parameterised, require extensive input data, and attempt to simulate both short-term and long-term dynamics of C in the soil (Petersen et al., 2002). Further, many simulation models are difficult to calibrate because of the issue of equifinality, meaning that different parameterisations provide similar fits to observed data (Beven and Freer, 2001). To simulate changes in SOC at farm- and regional-scales, models should require as few parameters as possible while still including the core mechanisms that regulate C turnover at the relevant timescale.

The C-TOOL model was developed to enable simulations of the medium- to long-term changes in SOC in temperate mineral soils under agricultural management, using fewer parameters and input data than the dynamic process-oriented models currently available. The model structure was inspired by the models presented by Petersen et al. (2002) and Saffih-Hdadia and Mary (2008), and shares many principles with other SOC turnover models, including CENTURY (Parton et al., 1987), CN-SIM (Petersen et al., 2005), Daisy (Hansen et al., 1991), ICBM (Andrén and Kätterer, 1997) and RothC (Coleman and Jenkinson, 1996). C-TOOL considers the inputs and turnover of C associated with three SOC pools in the topsoil (0–25 cm) and three corresponding pools in the subsoil (25–100 cm), the transport of SOC from topsoil to subsoil, and emissions of CO_2. Simulation of ^{14}C natural abundance is also facilitated. In this paper we report the parameterisation of the model using data from 19 treatments drawn from seven long-term field experiments in the United Kingdom, Sweden and Denmark.

2. Materials and methods

2.1. C-TOOL structure

Fig. 1 shows the compartment structure of C-TOOL. Our focus on medium- to long-term trends in SOC storage facilitates a relatively simple model structure. Thus different categories of organic inputs can be merged and the microbial biomass can be ignored as a separate C pool (Kätterer and Andrén, 1999). In contrast to the model framework presented by Petersen et al. (2002), the present C-TOOL model discriminates between SOC in topsoil (0–25 cm) and subsoil (25–100 cm), and includes vertical transport of C from topsoil to the subsoil. More complex simulation models seek to incorporate biological, chemical and physical processes known to occur in the soil and draw on state-of-the-art knowledge on soil organic matter composition and stabilisation. However, SOC pools in such simulation models do not yet correspond to specific and measurable fractions of soil organic matter even though some progress in this direction has been achieved (Christensen, 1996; Skjemstad et al., 2004; Sohi et al., 2001; Zimmermann et al., 2007).

The C-TOOL structure is built around three conceptual pools: C in fresh organic matter (FOM), C in humified organic matter (HUM), and C in resistant organic matter (ROM). Carbon enters the soil via addition of FOM in aboveground plant residues, roots and rhizodeposition, and a fraction of the organic matter in animal manure (see below). These inputs to FOM are all ascribed the same decomposition rate.

The HUM pool includes C in organic matter that has been subject to microbial transformation and has become physically and/or chemically stabilised in the soil. Since animal manure has been exposed to microbial transformation in the digestive tract and during subsequent storage, a fraction of the manure C is allocated directly to HUM. This is regulated by f_{HUM} (>0 for manure and 0 for plant residues). The C in the HUM pool is ascribed a decadal scale half-life.

The ROM pool contains C in organic matter that has been rendered biologically resistant by physico-chemical mechanisms. In C-TOOL, the ROM pool is assumed to have a very slow turnover. Most SOC turnover models include a compartment that is either considered biologically inert or has a very slow turnover time (Falloon and Smith, 2000), and ROM turnover is considered of little importance in simulations over one or two centuries (Andrén and Kätterer, 1997). Radiocarbon dating suggests that the smallest possible size of the ROM pool corresponds to ca. 10% of the SOC in topsoil (assuming that ROM is of almost infinite age) while the upper limit for ROM is ca. 50% of the SOC (Petersen et al., 2005). Using inverse modelling and data from six long-term bare fallow experiments, Barré et al. (2010) found the stable C pool to account for ca. 25% of the initial SOC content (Barré et al., 2010). Analyses of soil buried beneath a Bronze Age burial mound showed that ca. 30% of the original SOC had survived 3300 years under aerobic conditions (Thomsen et al., 2008a).

2.2. Transformations

Various factors affect the decomposition process, including the nature of the added organic matter and environmental factors such as soil temperature, water availability, pH and texture (Stockmann et al., 2013). In C-TOOL, the driving variables are soil texture (clay content), soil temperature, soil C/N ratio, and the type, quantity and application date of organic matter inputs. C-TOOL does not consider soil water as a limiting factor when simulating C turnover over decades to centuries but assumes that temperature is the overarching climatic driver for C turnover in the European temperate area from which data for parameterisation was retrieved. The model is therefore not applicable to soils exposed to prolonged dry seasons or water-logged soils.

Tillage is often assumed to enhance the turnover of SOC (Chatskikh et al., 2009), but a recent meta-analysis suggests that tillage does not affect total SOC stock but merely its distribution in the topsoil layers (Luo et al., 2010). Adopting the paradigm of simplicity, C-TOOL does not consider the effects of soil tillage intensity.

The turnover of C in each pool is described by first-order reaction kinetics:

$$\frac{dC_i}{dt} = -k_i C_i F_T(T) \tag{1}$$

where k_i is decomposition rate coefficient (yr^{-1}) for pool i at standard conditions (10 °C), C_i is the C content in pool i ($Mg\,C\,ha^{-1}$) and $F_T(T)$ is a temperature coefficient.

The temperature coefficient is modified to obtain unity at 10 °C in the following manner (Kirschbaum, 1995):

$$F_T(T) = 7.24 \exp\left[-3.432 + 0.168T\left(1 - \frac{0.5T}{36.9}\right)\right] \tag{2}$$

where T is temperature (°C).

Soil temperature at a given depth z (m) and time (t) is described using the function of Monteith and Unsworth (1990):

$$T(z,t) = \bar{T} + A(0)\exp\left(-\frac{z}{D}\right)\sin\left(\omega t - \frac{z}{D}\right) \tag{3}$$

where $\bar{T}$ is the average monthly air temperature (°C), $A(0)$ is the amplitude in air temperature at the soil surface on a monthly basis (°C), D is the damping depth (m), and ω is angular frequency of the harmonic oscillation in temperature, $2\pi/P$; P is period (the length of each cycle, or distance from one peak to the next).

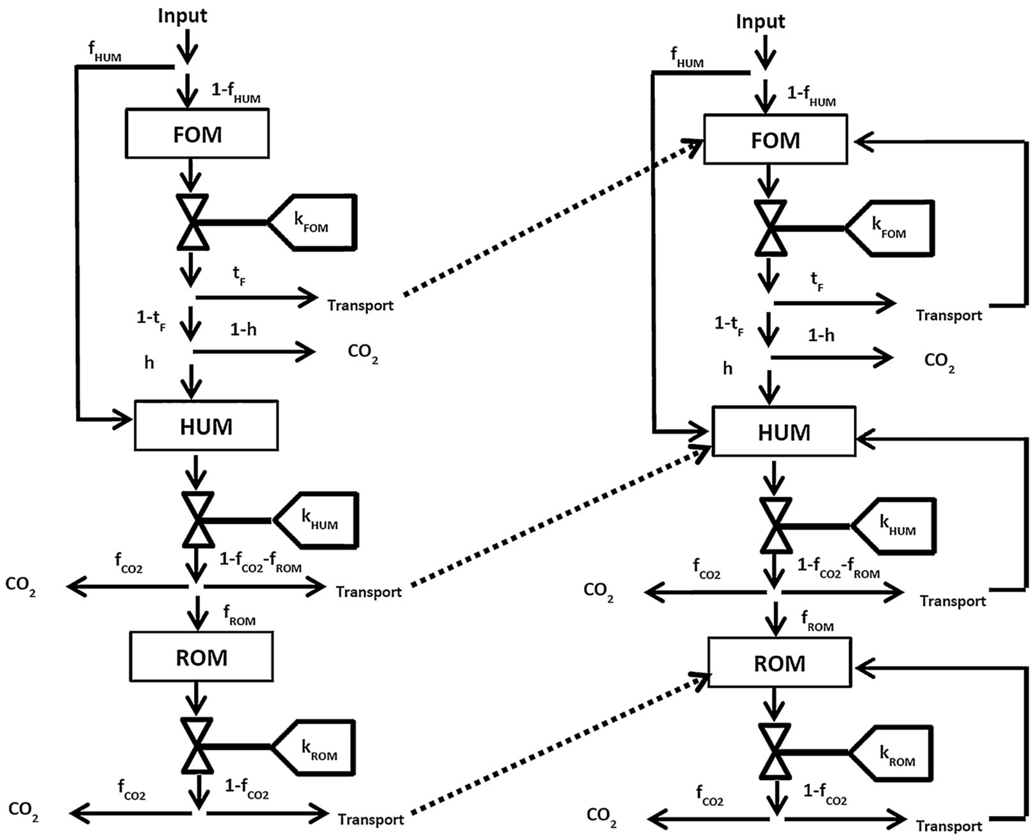

Fig. 1. C-TOOL model structure for top and subsoil; FOM: fresh organic matter, HUM: humified organic matter, ROM: resistant organic matter, f_{HUM}: fraction of input going to HUM (f_{HUM} is >0 for manure and 0 for plant residues), k_{FOM}: decomposition rate of FOM, k_{HUM}: decomposition rate of HUM, f_{ROM}: fraction of FOM going to ROM, k_{ROM}: decomposition rate of ROM, t_F: the fraction going to downward transport, h: humification coefficient, f_{CO_2}: fraction of released CO$_2$. *Note*: The rate constants and fraction are the same for both topsoil and subsoil.

After simulating the turnover of FOM, two steps are applied in C-TOOL: (1) a proportion (t_F) of the C is allocated to the subsoil, and (2) the remaining C undergoes humification (Fig. 1).

The clay content influences the humification coefficient (h), which is the proportion of C that is partitioned to the HUM pool (Fig. 1). The clay response function is from Coleman and Jenkinson (1996):

$$R = 1.67(1.85 + 1.6\exp(-7.86X)) \quad (4)$$

where R is the ratio (C lost as CO$_2$)/(C directed to HUM), and X is clay fraction in the soil (kg kg^{-1})

The constant 1.67 is used to adjust to observed values of R for all soils (Coleman and Jenkinson, 1996).

The humification coefficient (h) is then calculated as:

$$h = \frac{1}{R+1} \quad (5)$$

With this equation, the humification coefficient ranges from 0.148 in soil without clay to 0.244 in soil with 100% clay.

The amount of SOC that is removed either by transport to the subsoil or emitted as CO$_2$ from the HUM pool is calculated simultaneously after the decomposition process (Fig. 1). The same procedure is applied to the ROM pool.

The proportion of SOC initially present as ROM depends on the history of the soil. For example, podsolised heathlands in Denmark were regularly burnt and the charred C as well as the stable C in spodic horizons became incorporated into the topsoils when converted to agricultural land. Today, these soils show relatively high soil C/N ratios, indicating a larger fraction of ROM (Thomsen et al., 2008b). In C-TOOL, the C/N ratio is used to partition SOC between the HUM and ROM pools, using the function:

$$f(cn) = \min(56.2cn^{-1.69}, 1) \quad (6)$$

where cn is the C/N ratio. This function returns a value less than one when the C/N ratio is above a threshold value of 10.8. This threshold was determined from an independent dataset of Danish agricultural soils (Thomsen et al., 2008b).

2.3. *Vertical transport of SOC*

The C-TOOL model uses a one-way, convection type transport model for simulating vertical transport of C in the soil (Jenkinson and Coleman, 2008). This model represents a simplification of the transport patterns reported in previous studies (Bruun et al., 2007; Dörr and Münnich, 1989). In C-TOOL, the transport of C occurs from all topsoil pools (0–25 cm depth) to the corresponding subsoil pool (25–100 cm). The fraction of C transported from each pool is shown in Fig. 1. For the subsoil pools, the vertical transport of SOC is also calculated but the amount of SOC is brought back to the donating SOC pool.

2.4. *Simulation of ^{14}C abundance*

The abundance of ^{14}C is simulated by C-TOOL. Although long-term C turnover in soil involves some isotope discrimination (Christensen et al., 2011), this is disregarded in C-TOOL. Radiocarbon measurements (^{14}C) are presented as per cent modern C (pM)

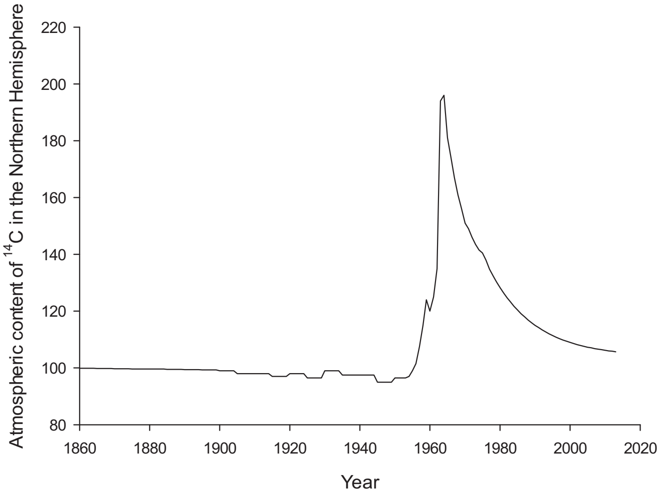

Fig. 2. Atmospheric content of ^{14}C in the Northern Hemisphere, taken as 100 per cent modern C (*pM*) in 1859 (Coleman and Jenkinson, 2008).

or as the difference in ^{14}C content relative to a defined standard (Δ^{14}C) (Petersen et al., 2002).

$$pM = 100\frac{\sum_n^{i=1}\lambda_i}{\sum_n^{i=1}C_i} \tag{7}$$

where λ_i is directly proportional to the amount of the isotope (^{14}C) in pool *i* and C_i is total C content in pool *i*.

$$\Delta^{14}C = 10(pM) - 1000 \tag{8}$$

Fig. 2 shows the historical atmospheric content of ^{14}C in the Northern Hemisphere. These were obtained from Coleman and Jenkinson (2008). Before 1860, C-TOOL assumes that the radiocarbon age of the plant material entering the soil each year is zero with values of 0 and 100 for Δ^{14}C and *pM*, respectively.

C-TOOL assumes the ^{14}C concentration in plant materials and animal manures, which enter the soil in a given year, to be the same as that in atmospheric CO_2. The ^{14}C values are given in units of "absolute" per cent modern (Stuiver and Polach, 1977). Thus the ^{14}C content in the C input for a given year is expressed as $pM/100$ or $(\Delta^{14}C + 1000)/1000$, i.e. taking the value for 1859 as 1.

2.5. *Implementation*

The C-TOOL components were assembled in MATLAB (MathWorks Inc., 2012). The program can utilise a range of time-steps for SOC contents. For C-TOOL simulations we used a monthly time step, applying mean monthly air temperature. For all datasets, the input of aboveground plant residues and root derived C was distributed over the year with 8% in April, 12% in May, 16% in June and 64% in July. Application of animal manures usually occurs in spring and/or autumn. In C-TOOL, animal manure application was taken to be in March. First-order relationships were integrated using the 4th order Runge–Kutta method (Abramowitz and Stegun, 1964).

2.6. *Long-term experiments and treatments*

Data for C-TOOL optimisation were extracted from long-term agricultural experiments located at three sites in Northwest Europe with different soil types and climatic condition (Table 1). The parameterisation was based on SOC data from 19 treatments drawn from experiments at Askov (Denmark), Rothamsted (UK) and Ultuna (Sweden). Concentrations of SOC in the topsoil had been measured in all treatments and amounts of SOC were calculated on an equivalent soil mass basis, using site-specific bulk density and a topsoil depth of 0–25 cm. One set of radiocarbon data from an Askov experiment was also employed.

2.6.1. *Askov, Denmark*

Askov Experimental Station is located at 55°28′ N and 09°07′ E with an annual precipitation of 862 mm and a mean annual temperature of 7.7 °C. The soil is a coarse sandy loam. Data were

Table 1
Summary of long-term treatments used for C-TOOL optimisation.

Treatment code used in this study	Site	Climate		Clay (%)	Treatment summary	Crops	Start and end of treatment
		Mean annual air Temperature (°C)	Mean annual precipitation (mm)				
ASK-FL1-B3	Askov, Denmark	7.7	862	12	Bare fallow	None	1956–1985
ASK-FL1-B4	Askov, Denmark	7.7	862	12	Bare fallow	None	1956–1983
ASK-FL2	Askov, Denmark	7.7	862	10	Bare fallow	None	1956–1987
ASK-GRASS	Askov, Denmark	7.7	862	12	NPK fertiliser	Grass mixture	1996–2002
ASK-UNF	Askov, Denmark	7.7	862	12	Unfertilised	Arable rotation	1894–present
ASK-1AM	Askov, Denmark	7.7	862	12	Animal manure	Arable rotation	1894–present
ASK-1NPK	Askov, Denmark	7.7	862	12	NPK fertiliser	Arable rotation	1894–present
BROAD-UNF	Rothamsted, UK	9.2	704	25	Unfertilised	Cont. winter wheat	1843–present
BROAD-MIN	Rothamsted, UK	9.2	704	25	NPK fertiliser	Cont. winter wheat	1843–present
BROAD-FYM	Rothamsted, UK	9.2	704	25	Farmyard manure	Cont. winter wheat	1843–present
HOOS-UNF	Rothamsted, UK	9.2	704	23	Unfertilised[a]	Cont. spring barley	1852–present
HOOS-FYM	Rothamsted, UK	9.2	704	23	Farmyard manure[a]	Cont. spring barley	1852–present
HOOS-FYM-UNF	Rothamsted, UK	9.2	704	23	Farmyard manure until 1871, then unfertilised[a]	Cont. spring barley	1882–present
ULT-UNF	Ultuna, Sweden	5.8	542	37	Unfertilised	Arable crops	1956–present
ULT-MIN	Ultuna, Sweden	5.8	542	37	Fertilised with $Ca(NO_3)_2$	Arable crops	1956–present
ULT-FYM	Ultuna, Sweden	5.8	542	37	Farmyard manure	Arable crops	1956–present
ULT-STR	Ultuna, Sweden	5.8	542	37	Unfertilised, straw incorporated	Arable crops	1956–present
ULT-MIN-STR	Ultuna, Sweden	5.8	542	37	Fertilised, straw incorporated	Arable crops	1956–present
ULT-FL	Ultuna, Sweden	5.8	542	37	Bare Fallow	Nil	1956–present

[a] From 1968 all HOOS treatments received a mean N rate of 72 kg N ha^{-1} yr^{-1}.

retrieved from four different experiments: The Askov Long-Term Experiments on Animal Manure and Mineral Fertilisers (Askov-LTE; Christensen et al., 2006) initiated in 1894 at the Lermarken site with four fields/blocks (B2, B3, B4 and B5), a bare-fallow (vegetation-free) experiment situated next to the B3- and B4-fields (ASK-FL1-B3 and ASK-FL1-B4, respectively) and running from 1956 to 1985 (Christensen, 1990; Christensen and Johnston, 1997), a small-plot bare-fallow experiment situated out-doors in concrete cylinders (ASK-FL2) and running from 1956 to 1986 (Christensen, 1988; Christensen and Johnston, 1997), and a field experiment with one- to six-years old grass-only ley (ASK-GRASS) also located at the Lermarken site (Christensen et al., 2009). In this experiment, plots with grass ley were established every year over a period of six years, the plots not yet in grass being sown to spring cereals. After six years, all grass leys (now 1- to 6-years old) were ploughed under and sown to spring cereals. Soil C was determined for individual leys when these were established and again when they were terminated.

The Askov-LTE data were extracted from three treatments in the B3-field: one kept unfertilised (ASK-UNF), one receiving mineral fertiliser (1 NPK) at a standard rate for the given crop (ASK-1NPK), and one receiving animal manure (1 AM) with a similar content of main nutrients (ASK-1AM). Radiocarbon data (*pM*) were extracted from same three treatments in the B2-field. This field has a different initial SOC level than the B3-field (Bol et al., 2005; Petersen et al., 2005). All SOC data refer to 0–20 cm soil depth and a dry bulk density of 1.55 g cm^{-3} was used throughout the study.

2.6.2. Rothamsted, United Kingdom

Rothamsted Research is located at 51°49′ N, 0°22′ W with an annual precipitation of 704 mm (1971–2000 mean) and a mean annual temperature of 9.5 °C. The soil is a silty clay loam. Data were extracted from two long-term field experiments: The Broadbalk Winter Wheat experiment (BROAD) initiated in 1843 and the Hoosfield Spring Barley experiment (HOOS) initiated in 1852. Three treatments in the Broadbalk experiment were considered (all applied since 1843): An unfertilised treatment (BROAD-UNF), a treatment receiving 144 kg N ha^{-1} yr^{-1} and standard rates of other plant nutrients (BROAD-MIN) and a treatment supplied with farmyard manure at an annual rate of 35 Mg ha^{-1} (BROAD-FYM). Yields are taken from the ‘continuous wheat’ Section 1 of the experiment, where winter wheat has been grown every year since 1843, except for occasional fallow years. Between 1926 and 1966, this section was fallowed approximately one year in five to control weeds, and neither manure nor fertiliser was applied. Three treatments in the Hoosfield experiment were included: an unfertilised treatment (HOOS-UNF), a treatment receiving farmyard manure each year 1852 to 1871 at an annual rate of 35 Mg ha^{-1} and no manure thereafter (HOOS-FYM-UNF), and a treatment receiving farmyard manure at an annual rate of 35 Mg ha^{-1} since 1852 (HOOS-FYM). In 1968 all Hoosfield treatments were subdivided into four plots to test different rates of fertiliser N (0, 48, 96 and 144 kg N ha^{-1} yr^{-1} as calcium ammonium nitrate). These rates change cyclically each year, so the mean N rate over each four year period is 72 kg N ha^{-1} yr^{-1}. The SOC was sampled to a depth of 23 cm at all Rothamsted treatments, and measured dry bulk densities ranged from 1 to 1.27 g cm^{-3} for BROAD and HOOS treatments. The initial SOC values (1843 for Broadbalk and 1852 for Hoosfield) have been estimated, and SOC in the FYM treatments has been adjusted for changes in soil bulk density (Johnston et al., 2009; Powlson et al., 2012). Broadbalk SOC data is shown for the ‘continuous wheat’ sections only. At Broadbalk, the subsoil SOC was measured in BROAD-UNF and BROAD-FYM (down to 69 cm depth in 1893) and BROAD-MIN (down to 91 cm depth in 1893 and 21–91 cm depth in 1999). In addition, dry bulk densities were measured at different depths in the subsoil of Broadbalk treatments (Dyer, 1902).

2.6.3. Ultuna, Sweden

The Ultuna long-term soil organic matter experiment was started in 1956 at Swedish University of Agricultural Sciences near Uppsala (59°82′ N, 17°65′ E). The mean air temperature is 5.8 °C and annual mean precipitation is 542 mm. The soil is a postglacial clay loam (Kirchmann et al., 1996).

Data were retrieved from six treatments: bare fallow (ULT-FL), an unfertilised treatment (ULT-UNF), a treatment given 80 kg N ha^{-1} in calcium nitrate (ULT-MIN), an unfertilised treatment with addition of straw (ULT-STR), a fertilised treatment (80 kg N ha^{-1}) with addition of straw (ULT-MIN-STR), and a treatment dressed with farmyard manure biannually (ULT-FYM) corresponding to 1.9 Mg C ha^{-1} yr^{-1}. In the straw-amended treatments 1.77 Mg C ha^{-1} yr^{-1} were added biannually (Kätterer et al., 2011). For the 3 years for which harvest was not quantified due to crop failure, the C input was assumed to be 50% of the average input from 2 years before and 2 years after. The SOC was sampled to a depth of 20 cm. All Ultuna treatments had the initial dry bulk density of 1.44 g cm^{-3}; however the bulk density differed between experimental treatments over time. The values of bulk density presented by Kätterer et al. (2011) were used to scale up the bulk density values throughout our study.

2.7. Climatic data

Daily data from meteorological stations at the experimental sites were used to calculate monthly mean temperature for the C-TOOL modelling.

2.8. Model parameterisation

C-TOOL contains several parameters that need to be estimated before the model can be applied (Fig. 1). The initial SOC content for each experiment and the HUM decomposition rate were optimised by minimising the squared difference between observed and simulated values (see below). For simplicity, we assumed that the initial SOC to a depth of 1 m was partitioned with 47% to the topsoil (0–25 cm) and 53% to the subsoil (25–100 cm) (Batjes, 1996).

The annual input of organic C to a soil arises from many sources, including aboveground crop parts shed during the growth period, stubble left after harvesting, and root-derived C deposited during and after the growth phase. The C input from aboveground crop residues can be determined by inverse modelling, crop modelling (Bruun et al., 2003) or by allometric relationships between yields and C input to the soil (Kätterer et al., 2011). The simplest approach is to use allometric relationships and this was used for the C-TOOL simulations. Dry matter yields for cereals were reported separately for grain and straw, whereas for other crops, only total above-ground mass was reported. Even when straw is harvested, a substantial fraction of the plant biomass is returned directly to the soil. In conventional farming, 50% of the C in total non-grain production may be returned, partly because these fractions are scattered as small particles or left in stubble and thus not removed after baling (Jørgensen et al., 2007). This was the case for Rothamsted treatments. For the field experiments at Askov and Ultuna, it was estimated that a quantity corresponding to 10% and 5% of the reported total above-ground biomass was recycled, respectively. The value for Ultuna is relatively small because at harvest, the aboveground biomass is cut close to the soil surface (Kätterer et al., 2011).

The belowground C inputs include dead roots and rhizodeposition. Gerwitz and Page (1974) assumed that root-derived C was the only input to soil below the plough layer (25 cm here) and that this input could be described by an exponentially decreasing depth distribution. According to Kätterer et al. (2011), 71% of the roots are allocated to the upper 20 cm, 80% to 30 cm and 85% to 40 cm.

Table 2
Values of carbon allocation to harvest (main and secondary products) and root and exudate C.

Crop	Harvest index of main crop relative to aboveground biomass (α)	Biomass of secondary crop product as proportion of yield of main crop product (δ)	Root and exudate C as proportion of total C assimilation (β)
Winter wheat (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000; Olesen et al., 2000)	0.45	0.55	0.25
Spring barley (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000)	0.45	0.55	0.17
Winter barley (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000)	0.39	0.55	0.17
Rye (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000; Kätterer et al., 2004)	0.38	0.80	0.25
Oat (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000)	0.40	0.60	0.17
Cereals for whole-crop harvest (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000; Lindroth and Båth, 1999)	0.75	0.00	0.17
Other cereals, mainly triticale (Danmarks-Statistik, 2004; Kuzyakov and Domanski, 2000; Kätterer et al., 2004)	0.38	0.80	0.25
Oilseed rape (Danmarks-Statistik, 2004; Kätterer et al., 2004)	0.37	0.90	0.25
Grass and grass-clover (Estimated from Christensen et al., 2009)	0.70	0.00	0.45
Potatoes (Andrén et al., 2004; Danmarks-Statistik, 2004)	0.70	0.00	0.11
Sugar beets (Andrén et al., 2004; Danmarks-Statistik, 2004)	0.70	0.00	0.12
Fodder beets (Andrén et al., 2004; Danmarks-Statistik, 2004)	0.70	0.34	0.12
Swedish turnip (Estimated from Andrén et al., 2004; Danmarks-Statistik, 2004)	0.70	0.00	0.12
Maize for silage (Estimated from Danmarks-Statistik, 2004)	0.85	0	0.15

Note: Several of the mentioned references were not primary studies; however their assumptions were used here.

The fraction of the root-derived C allocated to the topsoil (0–25 cm) depends on crop type and was fixed as 70% for autumn sown crops (Kätterer et al., 1993), 80% for spring sown crops (Hansson and Andrén, 1999), and 90% for grassland (Kätterer and Andrén, 1999). Values for carbon allocation to roots are crop specific and were derived from various studies (Table 2). The C concentration in plant dry matter assumed to be 45% in all crop parts. Using the parameters in Table 2, Table 3 shows the allometric calculations of total C deposition.

The composition of the different types of animal manure was available for some years at each site, and these data were used to estimate C inputs for the manured treatments. The fraction of the animal manure (f_{HUM}) that is transferred directly to the HUM pool (Fig. 1) was estimated using data from Stemmer et al. (2000), who examined soils to which a batch of ^{14}C labelled straw and ^{14}C labelled animal manure had been applied 30 years earlier. The soils were under crop rotations or kept bare fallowed. The ratio of ^{14}C to organic C content averaged over the treatments was 1:1.358 after 30 years. Considering the clay content dependent value of h (Equations 4 and 5), the f_{HUM} for animal manure was calculated as f_{HUM} = 1.358–1-h, providing f_{HUM} values for animal manure in the range 0.14–0.16 depending on soil clay content. The f_{HUM} for plant materials was set to 0.

Table 3
Calculations of total C (Mg ha^{-1}) deposited in the top- and sub-soil.

Parameters
α = Harvest index of main crop product relative to aboveground biomass
β = Root biomass and exudate C (below-ground C) as proportion of total net C assimilation
δ = Biomass of secondary crop product (e.g. straw) as proportion of yield of main crop product
ζ = Proportion of secondary crop product that is harvested
ε = Concentration of C in biomass DM (kg Mg^{-1})
ξ = Proportion of root and exudate C deposited in top soil (0–25 cm)

Input
Y_{main} = DM yield of main crop product (Mg DM ha^{-1})

C partitioning
C_{main} = C yield of main crop product = $\varepsilon Y_{\text{main}}$
C_{tot} = total C assimilation = $1/((1-\beta)\alpha)\,C_{\text{main}}$
The above-ground carbon in crop residues (C_{resid}) is calculated as:
If there is only one crop product or if the secondary product is not harvested:
$C_{\text{resid}} = (1/\alpha - 1)\,C_{\text{main}}$
If the secondary product is harvested:
$C_{\text{resid}} = (1/\alpha - 1 - \delta\zeta)C_{\text{main}}$
The below-ground carbon in root residues and exudates (C_{resid}) are calculated as:
$C_{\text{below}} = \beta C_{\text{tot}} = \beta/((1-\beta)\alpha)C_{\text{main}}$
The C in residues, roots and exudates deposited in topsoil (C_{rootTop}) is calculated as
$C_{\text{rootTop}} = C_{\text{resid}} + \xi C_{\text{below}}$
The C in residues, roots and exudates deposited in subsoil (C_{rootSub}) is calculated as
$C_{\text{rootSub}} = (1-\xi)C_{\text{below}}$
α, β and δ are defined in Table 2, ε = 0.45, ξ = 0.7 (winter crops), 0.8 (spring crops) or 0.9 (grassland).

Guenet *et al.* (2013) found that FOM decomposition rates may range from 0.2 to 10 yr^{-1}. In our study, the decomposition rate of the FOM pool (k_{FOM}, 1.44 yr^{-1}) was taken from Petersen et al. (2005). The initial fraction of SOC allocated to the topsoil ROM pool was 0.405 and the decomposition rate of ROM pool (k_{ROM}) was set to 4.63×10^{-4} yr^{-1} so that the simulated ^{14}C age of Askov soils equals that of the "pre-bomb" measurements. The fraction of topsoil HUM partitioned to the ROM pool (f_{ROM}) was set to 0.012, a value that under steady state conditions maintains the fraction of SOC in the ROM pool at 0.405 (Petersen et al., 2005).

The fraction of topsoil FOM transported to the subsoil is expressed by the parameter t_F. In a study with ^{14}C labelled ryegrass, Jenkinson and Rayner (1977) found that 0.40–0.75% of the labelled C was leached over a period of two years. Using ^{14}C labelled barley straw, Sørensen (1987) observed that 9–10% of the labelled C that was retained in the soil after 8 years was residing in the subsoil, i.e. below 20 cm. On the basis of this span, a tentative value of t_F = 0.03 is utilised in C-TOOL. For the HUM and ROM pools, a fixed proportion (f_{CO_2}) of the decomposed C is emitted as CO$_2$. The value for f_{CO_2} was set to 0.628.

The two remaining C-TOOL parameters; i.e. the decomposition rate of HUM (k_{HUM}) and the total initial soil C content in the long-term treatments were estimated by simultaneous optimisation, utilising a Marquard–Levenberg algorithm (Marquard, 1963). The optimisation was performed with a weighted squared error sum as the target function, using measured topsoil SOC data and the corresponding simulated data. The initial distribution of SOC between HUM and ROM pool influences C-TOOL simulations (Bruun and Jensen, 2002), but this distribution cannot be related to measurable entities. The procedure used when optimising the initial SOC content and k_{HUM} was to begin the simulations with an initialisation

Table 4
C-TOOL parameters and values.

C-TOOL parameter	Value
Initial C content (Mg ha^{-1})	Optimised for each treatment
Initial f_{HUM} (top and sub soil)	0.595
Initial f_{ROM} (top and sub soil)	0.405
f_{HUM} (Crop)	0
f_{HUM} (FYM)	1.358–1-h
f_{ROM}	0.012
k_{FOM} (yr^{-1})	1.44
k_{HUM} (yr^{-1})	0.0192 ± 0.008[a]
k_{ROM} (yr^{-1})	4.63×10^{-4}
t_F	0.03
f_{CO_2}	0.628

[a] Standard error.

period of 30 years i.e. prior to the period for which measurements were available. For each treatment, the total SOC at the start of the initialisation period was optimised on the measured value at the start of the experiment, with the condition that the partitioning of SOC between pools was: FOM, 0; HUM, 0.595; and ROM, 0.405 (see above). The first five years of management applied to treatments amended with mineral fertilisers was repeated six times in the initialisation period. The exceptions were: (1) the ASK-GRASS treatment where information on the management (spring cereals amended with mineral fertilisers and straw removal) preceding the experimental treatment was available (Christensen et al., 2009), and (2) the Broadbalk and Hoosfield experiments where the unfertilised wheat and spring barley and straw removal were considered as the management in initialisation period. The weighted target function, as well as the other procedures for optimisation, was taken from Petersen et al. (2005). The target function T was calculated as:

$$T = \sqrt{\frac{\sum_i^m \sum_j^{n_i} \sum_k^{l_{ij}} ((O_{ijk} - S_{ijk})^2)/(l_{ij} O^2_{\bar{j\ldots}})}{n}} \qquad (9)$$

where i sums over all measurement types, j sums over all data series within each type, O_{ijk} is observation k in experiment j of type i, S_{ijk} is simulation k in experiment j of type i, $O_{\bar{j\ldots}}$ is average of all observation of type i and l_{ij} is total number of observations of type i in data series j.

Optimisation was performed using a nonlinear curve-fitting function according to Eq. (9) in MATLAB (MathWorks Inc., 2012). A lower and upper boundary for each parameter and fraction was defined prior to the start of optimisation using information from previous studies (Jenkinson and Rayner, 1977; Kätterer et al., 2011; Petersen et al., 2005). Then, optimisation was run iteratively until all parameters stabilised by minimising the sum of root mean squared errors (RMSE) locally. The C-TOOL model parameters and their default and optimised values are shown in Table 4.

2.9. Statistical analysis

Different statistical metrics were used to compare the simulated and observed topsoil SOC storage (Mg ha^{-1}) for each experimental site. The comparison was made by calculation and evaluation of the mean bias error (MBE), root mean square error (RMSE), coefficient of determination (R^2) and model efficiency (EF). Statistical analysis was performed using MATLAB (MathWorks Inc., 2012). MBE evaluates the difference between the mean of the model-simulated variable and the observed variable, and provides an indication of the bias in the simulation (Willmott, 1982).

$$\mathrm{MBE} = \frac{\sum_n^{i=1} (P_i - O_i)}{n} \qquad (10)$$

where O_i is the measured value, P_i is the simulated value and n is the number of paired values. Ideally a zero value of MBE should be obtained while a positive and a negative value indicates overestimation and under-estimation, respectively.

The difference between the simulated and the measured values were calculated as the root mean square error, RMSE (Smith et al., 1997).

$$\mathrm{RMSE} = \sqrt{\sum_{i=1} \frac{(P_i - O_i)^2}{n}} \qquad (11)$$

To assess whether simulated values follow the same pattern as measured values, the sample coefficient of determination (R^2), can be calculated as below (Smith et al., 1997).

$$R^2 = \left(\frac{\sum_n^{i=1} (O_i - \bar{O})(P_i - P)}{((\sum_n^{i=1} (O_i - \bar{O})^2)^{1/2} ((\sum_n^{i=1} (P_i - \bar{P})^2)^{1/2}} \right)^2 \times 100 \qquad (12)$$

where $\bar{O}$ and $\bar{P}$ are the mean of measured and simulated values, respectively.

Model efficiency (EF) provides a comparison of the efficiency of describing the data compared to just using the mean of all observations. Model efficiency values range from 1 (perfect model) to negative infinity. Negative values indicated that the average of all measured values was a better estimator than the model (Smith and Smith, 2007).

$$\mathrm{EF} = \frac{\sum_n^{i=1} (O_i - \bar{O})^2 - \sum_n^{i=1} (P_i - O_i)^2}{\sum_n^{i=1} (O_i - \bar{O})^2} \qquad (13)$$

3. Results

The C-TOOL simulations for the Askov bare fallow and grassland treatments are shown in Fig. 3 and the results from the Askov-LTE treatments in Fig. 4. Table 5 shows the partitioning of SOC among C-TOOL pools at onset and at the end of the simulated periods.

With the exception of the ASK-1AM and ASK-GRASS treatments, a loss of topsoil C was simulated at Askov. The mean annual loss was 0.6 Mg C ha^{-1} in bare fallow treatments (ASK-FL1-B3, ASK-FL1-B4, and ASK-FL2) and 0.2 and 0.1 Mg C ha^{-1} in ASK-UNF and ASK-1NPK treatment, respectively. An annual increase of approximately 0.9 Mg C ha^{-1} was simulated for topsoil of the ASK-GRASS treatment. At Askov, the simulations of subsoil C showed a decrease in bare fallow, ASK-UNF, ASK-1AM and ASK-1NPK (Table 5), while subsoil C increased 1 Mg C ha^{-1} yr^{-1} in the ASK-GRASS treatment. The simulations for the ASK-1AM treatment showed no change in topsoil C storage; however, simulated changes in topsoil C of ASK-1NPK and ASK-1AM did not concur with measured values (Fig. 4b and c).

The measured and simulated ^{14}C values of the B2-field are shown in Fig. 4(d, e and f). The initial ^{14}C values in soil from all three treatments were below 100 *pM*. The testing of thermonuclear weapons in the atmosphere, which peaked in 1963, nearly doubled the atmospheric concentration of ^{14}C (Fig. 2). This increase in atmospheric ^{14}C was subsequently traced in soil from B2-field treatments. The ^{14}C content simulated with C-TOOL aligned with measured values during the period where the bomb-derived pulse of atmospheric ^{14}C was incorporated into the soil. In the subsequent period, simulated ^{14}C values were higher than measured ones. The measured and simulated ^{14}C content was higher in soil amended with animal manure (Fig. 4e) than in soil kept unfertilised and mineral fertilised soil (Fig. 4d and f).

The simulated topsoil C in the Rothamsted treatments is shown in Fig. 5. At Broadbalk, the model simulated a small loss of topsoil C in BROAD-UNF (0.1 Mg ha^{-1} yr^{-1}) while measurements show

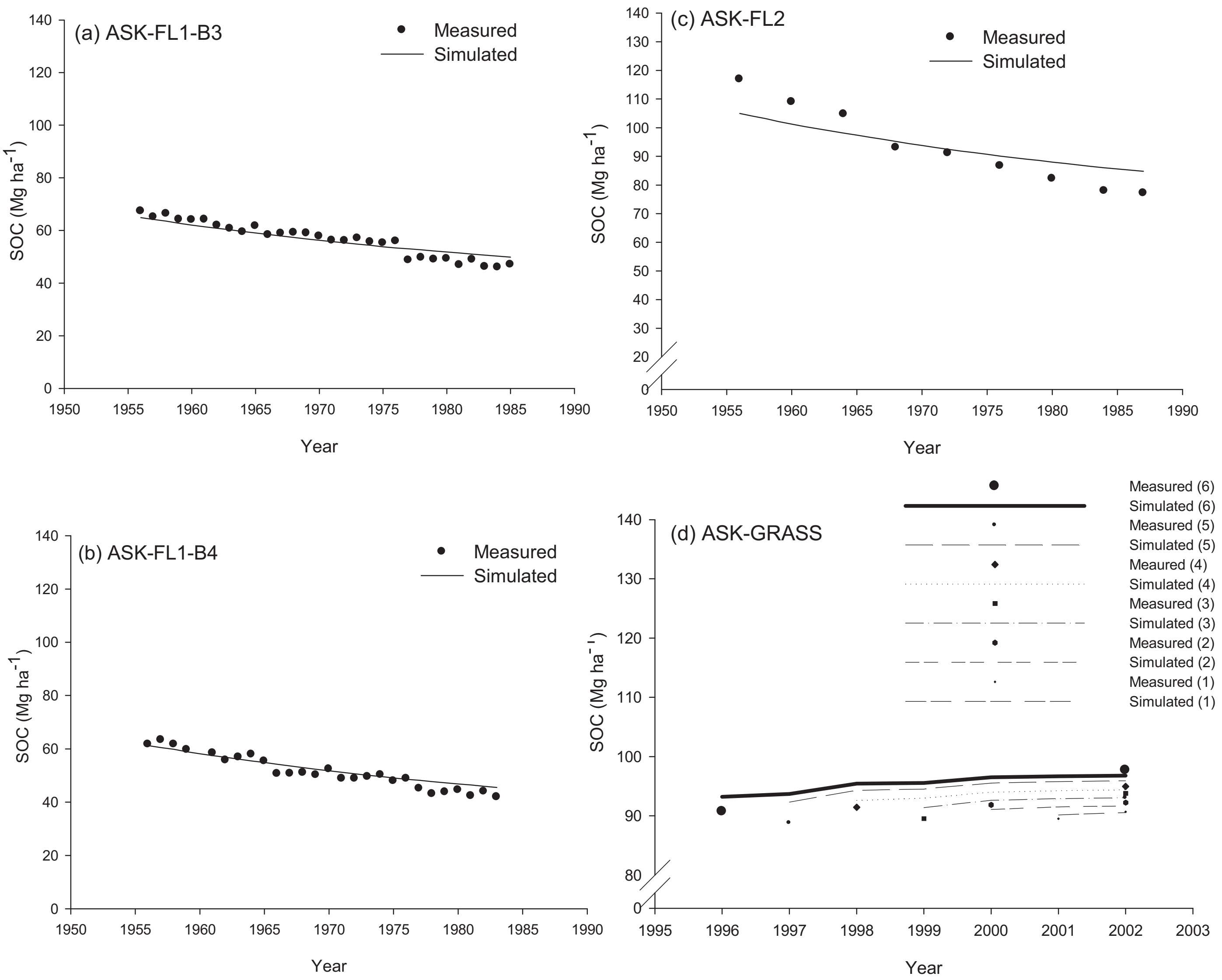

Fig. 3. Measured and simulated SOC content at 0–25 cm depth in bare fallow (a, b, and c) and grassland (d) treatments in Askov, Denmark. *Note*: The numbers in parenthesis in (d) show the age of grass leys (from 1 to 6 years). The thickest line and symbol indicate the oldest grass ley.

no change. The model simulated little change of topsoil SOC in BROAD-MIN and an increase in BROAD-FYM of 1 Mg C ha^{-1} yr^{-1} during the first 20 yrs., and then around 0.2 Mg C ha^{-1} yr^{-1} during 1863–2010. The simulated results are in agreement with previous measurements (Powlson et al., 2012). In Hoosfield, the simulation for HOOS-UNF showed a decrease in topsoil C (0.1 Mg ha^{-1} yr^{-1}) during the simulated period. For HOOS-FYM, SOC increased by 0.2 Mg ha^{-1} yr^{-1} while the HOOS-FYM-UNF treatment lost topsoil C at a rate of 0.2 Mg C ha^{-1} yr^{-1}, once FYM was no longer applied. Simulations for subsoil C at Rothamsted showed a decrease in the BROAD-UNF, HOOS-UNF and HOOS-FYM-UNF treatment whereas an increase in subsoil C was simulated for BROAD-MIN, BROAD-FYM and HOOS-FYM (Table 5). The subsoil organic C contents at different depths were measured in three treatments in Broadbalk in 1893 and also one treatment and one depth in 1999. In 1893, the 23–69 cm layer of BROAD-UNF, BROAD-MIN and BROAD-FYM contained 29, 30 and 35 Mg C ha^{-1}, respectively (after Dyer, 1902), while the 23–91 cm layer of BROAD-MIN contained 42 Mg C ha^{-1} (Jenkinson et al., 2008). The corresponding simulated subsoil C storage was 36, 44 and 52 Mg C ha^{-1} in 25–100 cm layer of BROAD-UNF, BROAD-MIN and BROAD-FYM, respectively. In 1999, the measured subsoil C content in the 23–91 cm layer of BROAD-MIN was 49 Mg C ha^{-1} (Jenkinson et al., 2008) while C-TOOL simulated 54 Mg C ha^{-1} in the 25–100 cm layer.

The C-flows simulated for 2010 by C-TOOL was compared for BROAD-UNF and BROAD-FYM treatments. The simulated SOC pools and C flows for BROAD-UNF treatment were: 20 Mg C ha^{-1} in topsoil, 31 Mg C ha^{-1} in subsoil, 1 Mg C ha^{-1} yr^{-1} emitted as CO_2 from topsoil and subsoil, and 0.1 Mg C ha^{-1} yr^{-1} transported from topsoil to subsoil. The corresponding values for BROAD-FYM were: 72 Mg C ha^{-1}, 73 Mg C ha^{-1}, 8 Mg C ha^{-1} yr^{-1}, and 0.6 Mg C ha^{-1} yr^{-1}.

C-TOOL simulations for topsoil C in 0–25 cm showed a good fit with measured data at Ultuna. The treatments ULT-FL, ULT-UNF, ULT-MIN and ULT-STR showed losses of topsoil C corresponding to 0.4, 0.3, 0.2 and 0.1 Mg C ha^{-1} yr^{-1}, respectively (Fig. 6). However, SOC increased in topsoil of ULT-FYM (0.1 Mg C ha^{-1} yr^{-1}). The simulation of SOC in the ULT-MIN-STR treatment showed almost no change in topsoil C. In Ultuna, subsoil C decreased in ULT-FL, ULT-UNF, ULT-MIN, ULT-FYM and ULT-STR during the simulation period; however, this was not the case for ULT-MIN-STR treatment (Table 5).

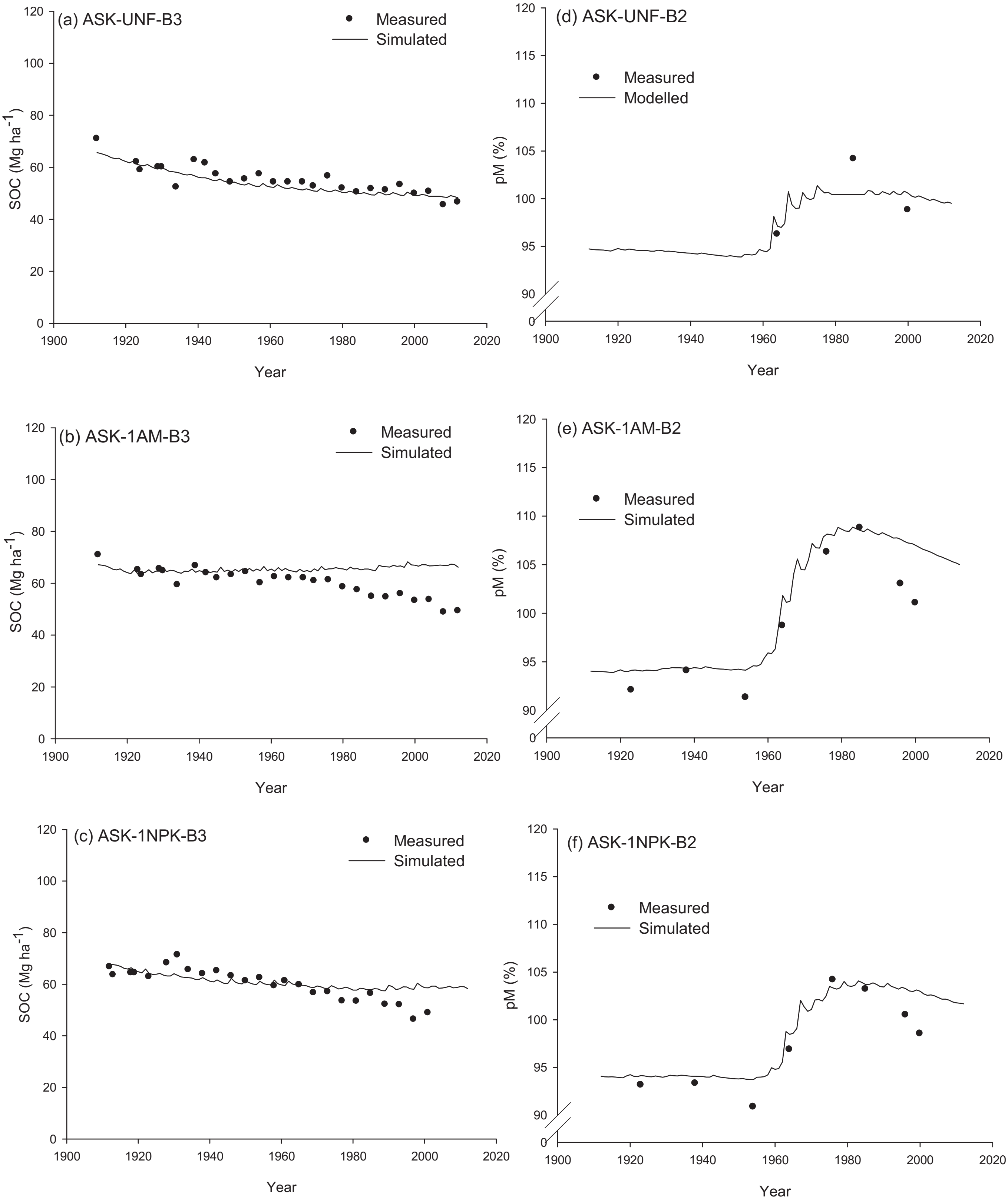

Fig. 4. Measured and simulated SOC content at 0–25 cm depth in different treatments of Askov B3-field crop rotations (a, b and c); Measured and simulated ^{14}C content at 0–25 cm depth in different treatments of Askov B2-field crop rotation (d, e, and f). *Note*: The different units on *y* axis.

Table 5
The size of C-TOOL simulated SOC pools (Mg C ha^{-1}) in the topsoil (0–25 cm) and subsoil (25–100 cm) at the first year of initialisation, onset and end of simulation runs of various treatments at Askov, Rothamsted, and Ultuna. ASK-FL2 and ASK-GRASS not included.

Treatment	Year	Topsoil			Subsoil		
		FOM	HUM	ROM	FOM	HUM	ROM
ASK-FL1-B3	0	0.2	28.1	37.1	0.2	44.8	42.4
	30	0.0	13.2	36.6	0.0	31.7	42.5
ASK-FL1-B4	0	0.2	31.4	30.2	0.2	50.7	34.6
	30	0.0	15.5	29.9	0.0	36.7	34.8
ASK-UNF	0	0.3	31.3	41.7	0.3	49.2	47.7
	119	0.1	8.7	39.3	0.1	23.2	47.9
ASK-1AM	0	0.3	31.3	41.7	0.3	49.2	47.7
	119	0.3	25.9	39.7	0.3	40.8	48.1
ASK-1NPK	0	0.3	31.3	41.7	0.3	49.2	47.7
	119	0.3	18.2	39.5	0.3	39.4	48.1
BROAD-UNF	0	0.1	13.5	17.9	0.1	25.1	20.6
	168	0.1	4.4	16.0	0.1	10.1	20.6
BROAD-MIN	0	0.1	13.5	17.9	0.1	25.1	20.6
	168	0.4	17.9	16.4	0.5	33.4	21.3
BROAD-FYM	0	0.1	13.5	17.9	0.1	25.1	20.6
	168	0.6	52.9	18.2	0.3	50.9	22.0
HOOS-UNF	0	0.1	14.8	20.7	0.1	27.7	23.8
	159	0.1	3.0	18.6	0.1	7.2	23.7
HOOS-FYM	0	0.1	14.8	20.7	0.1	27.7	23.8
	159	0.6	51.3	20.7	0.4	48.8	25.1
HOOS-FYM-UNF[a]	0	0.1	14.8	20.7	0.1	27.7	23.8
	159	0.1	5.3	19.0	0.1	12.7	24.1
ULT-FL	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.0	7.2	24.7	0.0	24.0	29.3
ULT-UNF	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.1	12.1	24.8	0.1	31.8	29.4
ULT-MIN	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.1	17.0	24.9	0.1	39.4	29.5
ULT-FYM	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.2	38.0	25.1	0.2	42.5	29.5
ULT-STR	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.7	24.5	24.9	0.3	45.2	29.5
ULT-MIN-STR	0	0.3	28.9	25.3	0.3	46.9	29.1
	54	0.8	29.7	25.0	0.4	53.1	29.6

[a] *Note*: HOOS-FYM-UNF treatment was started from 1882. The HOOS-FYM-UNF treatment was for a shorter period, and started at a much high SOC level than the other two HOOS treatments, as it had received FYM from 1852 to 1871. For consistency, year 1852 was considered year 1 for all HOOS treatments.

Statistical analysis was performed not for individual treatments but for each site, whereby the degrees of freedom and hence the robustness of the analysis were increased (Table 6). The MBE values ranged from -5.58 to 0.68 Mg C ha^{-1}, and the RMSE values ranged from 4.64 to 8.86 Mg C ha^{-1}. Values for R^2 were equal to or above 90 for all three sites, indicating a satisfactory overall agreement between simulated and measured values. The EF value was positive for all the experimental sites.

Table 6
Values of MBE, RMSE (%), R^2 and EF for simulated and measured topsoil C of each experimental site.

Experimental site	MBE	RMSE	R^2	EF
Askov, Denmark	0.68	4.76	92.33	0.85
Rothamsted, UK	-5.58	8.86	94.93	0.83
Ultuna, Sweden	-0.48	4.64	90.00	0.81

MBE: mean bias error; RMSE: root mean square error; R^2: coefficient of determination; EF: model efficiency.
The number of observations were 146, 63 and 114 in Askov, Rothamsted and Ultuna; respectively.

4. Discussion

4.1. Topsoil C

The C-TOOL estimates showed satisfactory fits to measured topsoil organic C in most of the treatments considered in this study (Figs. 3–6). The best fits were obtained for bare-fallow soil (except ASK-FL2) and soil kept unfertilised (except BROAD-UNF). The major discrepancy between measured and modelled topsoil C found for the bare-fallow treatment ASK-FL2 may be ascribed to the set-up of this experiment. The ASK-FL2 was a small-plot experiment based on topsoil that was retrieved from permanent grassland and coarsely sieved before being placed in the cylinders (Christensen, 1988). This soil with a high initial content of labile SOC showed a steeper decline in SOC than was modelled by C-TOOL. The more intense turnover of SOC could not apparently be captured by C-TOOL with its present parameterisation, and the initialisation run did not match the measured initial SOC storage in the pre-fallow grassland soil. In contrast, the two field-based bare-fallow experiments ASK-FL1-B3 and ASK-FL1-B4 (Christensen, 1990) had a long

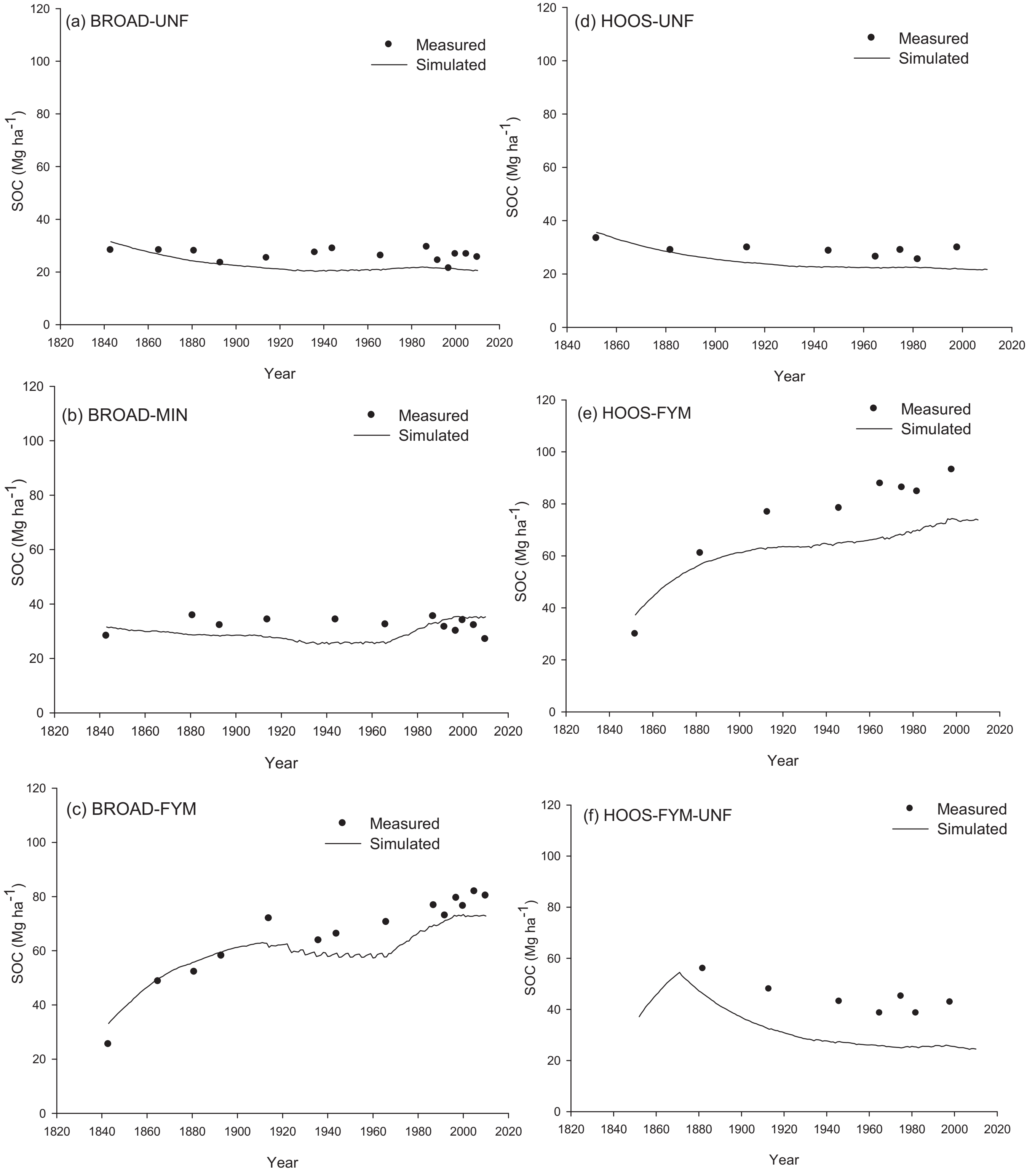

Fig. 5. Measured and simulated SOC content at 0–25 cm depth in Broadbalk (a, b, and c) and Hoosfield (d, e, and f) experiments in Rothamsted, United Kingdom.

history of arable four-course rotations with removal of harvestable plant biomass and thus a much smaller initial content of labile SOC.

Simulated and measured values for topsoil C in the ASK-1AM and ASK-1NPK treatments diverged from around 1970 and onwards (Fig. 4). In the ASK-1AM treatment, conventional farmyard manure (FYM) was applied from 1894 to 1922. From 1923 to 1972, the FYM was supplemented with liquid manure (LM), and then in 1973, addition of FYM and LM was replaced by cattle slurry (Christensen et al., 2006). One contributing factor to the discrepancy between simulated and measured SOC in ASK-1AM could be the effect of manure type on f_{HUM}. This fraction was derived from results of Stemmer et al. (2000) who studied the stabilisation of FYM-derived C in soil. Future C-TOOL simulations may benefit from improving the estimation of f_{HUM} to account for different types of manure. At Rothamsted and Ultuna, FYM was used throughout the experimental periods. This probably contributed to the better fit

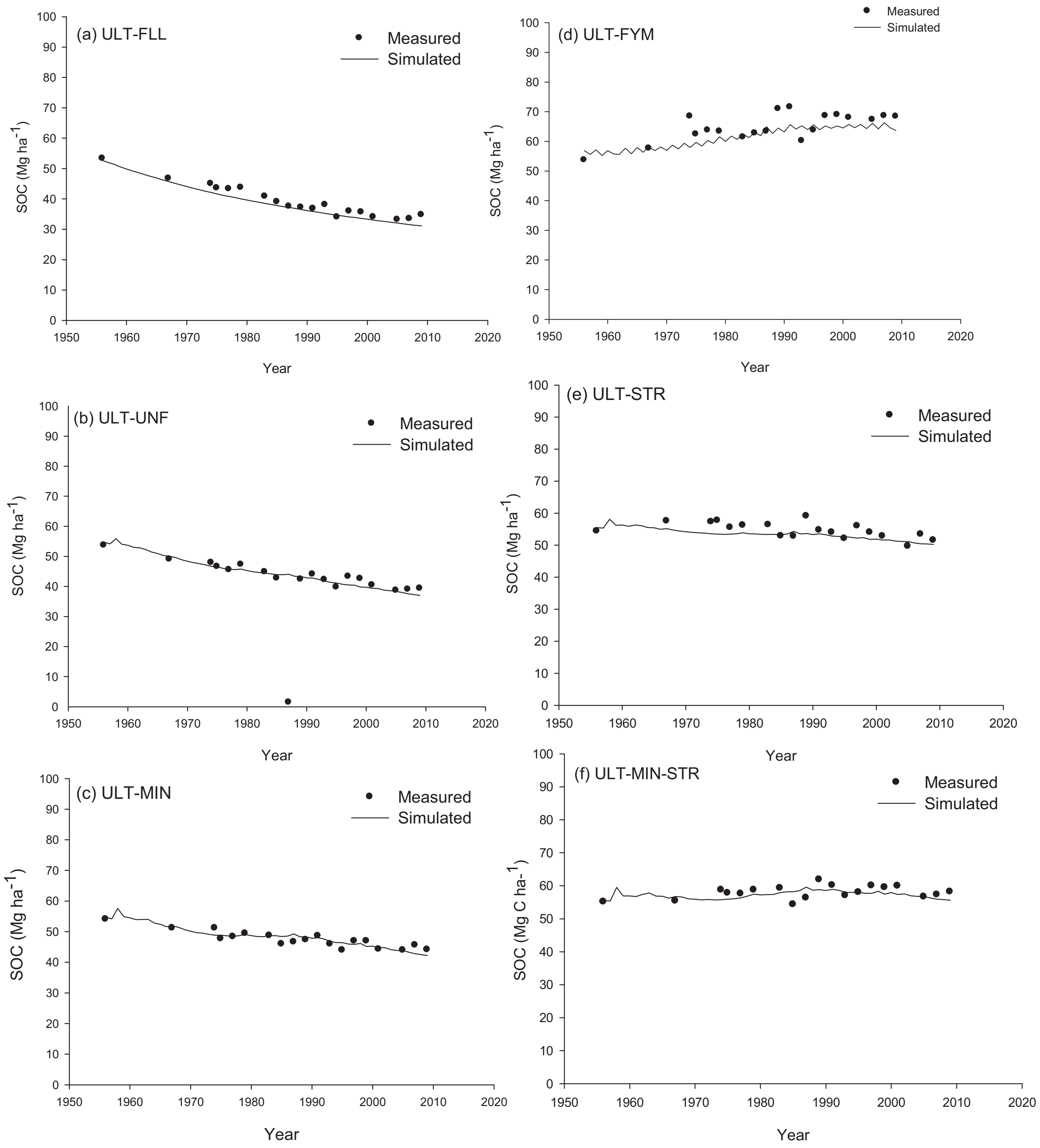

Fig. 6. Measured and simulated SOC content at 0–25 cm depth in the different treatments at Ultuna, Sweden.

of the simulation for manured treatments at these experimental sites.

Calculations of the cumulated input of C from the crop to the topsoil involved the use of allometric functions. This approach has the advantage of simplicity and enables the model to be used in situations where the only available crop data are crop types and yields of harvested biomass. This advantage is likely to be obtained at the cost of substantial uncertainty regarding C inputs in the form of plant biomass shed during the growth phase, non-recoverable harvest residues, stubble, and belowground deposition. In particular estimates of annual inputs of root-derived C are associated with substantial uncertainties. Deposition of C in macro-roots has been found to be independent of aboveground production and thus not responsive to higher crop yield (Chirinda et al., 2012), and Kuzyakov and Domanski (2000) suggested that the portion of assimilated C allocated belowground decrease with increased N fertilisation. This may partly explain the divergence between measured and simulated values for both ASK-1AM and ASK-1NPK treatment, since the improved crop yields obtained in these treatments since 1972 (Christensen et al., 2006) may not have led to higher inputs of root-derived C as assumed by the allometric approach (Bolinder et al., 2007; Chirinda et al., 2012). C-TOOL applies fixed values for harvest index and the ratio of above to belowground C for individual crops which may be less realistic, recalling the historic progress in plant breeding towards higher production potentials and more favourable harvest indices, and the development of efficient crop protection measures (Shearman et al., 2005). Although similar improvements in crop productivity have occurred in the Rothamsted treatments, the C-TOOL simulations showed a better fit with observed topsoil SOC at this site.

C-TOOL simulates topsoil C in 0–25 cm soil whereas soil for SOC determination was sampled in 0–20 cm at Askov and Ultuna and 0–23 cm at Rothamsted. The measured values were converted to SOC in 0–25 cm by assuming the same C concentration in 0–25 cm as found in the sampled soil. The model estimates were not converted from simulated depth back to original soil sampling depth.

4.2. Subsoil C

It is well recognised that subsoils (30–100 cm) typically store about 50% of the SOC found in the 0–100 cm soil profile (Batjes, 1996), but the impact of agricultural management is generally considered to affect only SOC stored in the topsoil. However, accumulating evidence from monitoring programmes shows that agricultural management may have decadal scale impacts also on SOC storage in subsoils (e.g. Taghizadeh-Toosi et al., 2014). While most simulation models do not explicitly consider SOC turnover in subsoils, C-TOOL was developed to encompass the vertical distribution of SOC down to 1 m. In simulation models that explicitly include subsoil SOC (e.g. RothPC-1; Jenkinson and Coleman, 2008), the basic mechanisms that regulate SOC turnover is taken to be the same for topsoil and subsoil SOC pools. This is also true for C-TOOL. However, there is accumulating evidence that the turnover of SOC in topsoil and subsoil is subject to different regulatory mechanisms (Fontaine et al., 2007; Salomé et al., 2010), and that the vertical transport of labile and stable SOC in the soil profile also differ (Braakhekke et al., 2013; Guenet et al., 2013). Different processes such as leaching of dissolved and particulate organic matter, bioturbation as well as stratified root inputs and differential C turnover may affect C contents down the soil profile (Rumpel and Kögel-Knabner, 2011). It has been indicated that root litter is a dominant source of subsoil SOC and also that roots may contribute more to refractory SOC pools than above-ground residues (Kätterer et al., 2011).

In our study, C-TOOL was used to simulate SOC content down to 1 m depth, but C-TOOL was optimised on the measured data for the topsoil only. Indeed, optimisation on the topsoil as well as subsoil dataset may improve the prediction of SOC storage. The lack of experimental data on changes in subsoil C storage obviously hampers a proper evaluation of the ability of C-TOOL to simulate subsoil C turnover. The few data from the Broadbalk experiment are not sufficient. We note, however, that the simulation of SOC in subsoil showed a decrease of SOC in the bare fallow and unfertilised treatments while most of the manured, fertilised and grassland treatments showed an increase in subsoil SOC storage. However, verification of management effects on subsoil C storage, subsoil C inputs from roots, vertical transport of C in the soil profile, and verification of different regulatory mechanisms for C turnover in subsoils should be given high priority.

5. Perspectives and conclusions

Compared to other SOC simulation models such as RothC, Daisy and CENTURY, C-TOOL requires fewer parameters and inputs. In our study, the C-TOOL model efficiency was above 0.8 for topsoil in all three sites. Farina *et al.* (2013) used RothC to simulate topsoil C storage for selected treatments in the Rothamsted Broadbalk Continuous Wheat experiment and found a model efficiency of 0.98. With C-TOOL we obtained a model efficiency of 0.83. However, the clay response function in RothC and C-TOOL needs to be modified based on the results from a recent meta-analysis study (Liu et al., 2014). Whether the trade-off between model efficiency and demand for input data and parameterisation is acceptable will depend on the purpose of the simulations. When the focus is to simulate farm- and regional-scale effects of management on medium to long term storage of SOC in temperate well-drained mineral soils, we consider C-TOOL to be a valid alternative to using a more complex model with default values for parameters, in situations where these would be expected to vary among locations.

Soil moisture is not considered as an important driving variable for SOC turnover in C-TOOL. We acknowledge that soil moisture remains a driver in the short-term dynamics of SOC on well-drained mineral soils with topsoils being particularly prone to fluctuations in soil water content. However, lack of biologically available soil water in temperate soils is usually a short-term phenomenon (days to weeks) that occurs in periods where temperature is not restricting decomposition rates. Thus most of the added organic matter (FOM) will be decomposed within a year, irrespective of intermittent short-term periods of reduced soil moisture. Sustained periods with lack of biologically available water may slow down the annual turnover of HUM and ROM but is also likely to decrease the net primary production and hence the input of crop C to the soil. The net result of these two opposing effects of water restriction is uncertain but would tend to reduce the sensitivity of the SOC dynamics to drought. We note that when analysing the underlying drivers of SOC variability with a set of reduced complexity models, Todd-Brown et al. (2013) concluded that soil moisture did not play an important role as a driving variable for soil C at the global and biome scales whereas temperature was important.

A number of spatially and temporally complex processes have been simplified greatly in C-TOOL, to provide a dynamic and deterministic description of SOC flows and transformations while making modest demands for input data and parameterisation. We have chosen to make most model parameters site-independent. The information required to run the model therefore consists of the initial C content of the soil, the monthly air temperature, the inputs of manure and straw C, and information on the crops grown and their yields. The modest demand for data also means C-TOOL offers a practical and low cost tool for estimating changes in soil C stocks at farm, regional and national scales allowing farmers and policy makers to evaluate effects of different options and scenarios for agricultural land use and management on soil C. The simplified structure, the method for estimating C inputs and the site-independent estimation of parameters adds some uncertainty to the predictions. Nevertheless, the statistical analysis and the visual evaluation of measured and modelled trend of topsoil SOC indicated that C-TOOL largely follows observed long-term SOC trends. C-TOOL provides a promising tool to estimate SOC change in well-drained mineral soils, in response to changes in climate or land use and management.

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