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

3

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23 **Highlights**

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25 • Our simple model (C-TOOL) was developed for well-drained mineral soils in Northwest
26 Europe.

27 • A number of spatially and temporally complex processes have been simplified greatly in C-
28 TOOL.

29 • The focus of C-TOOL is on long-term trends for soil organic carbon content.

30 • The simple model structure facilitates calibration and requires few inputs.

31 • A decline in soil organic carbon was simulated in most soils under agricultural management,
32 except those associated with large inputs of C from grassland and animal manure.

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47 **Abstract**

48 Soil organic carbon (SOC) is a significant component of the global carbon (C) cycle. Changes in
49 SOC storage affect atmospheric CO₂ concentrations on decadal to centennial timescales. The C-
50 TOOL model was developed to simulate farm- and regional-scale effects of management on
51 medium- to long-term SOC storage in the profile of well-drained agricultural mineral soils. C-
52 TOOL uses three SOC pools for both the topsoil (0-25 cm) and the subsoil (25-100 cm), and applies
53 temperature-dependent first order kinetics to regulate C turnover. C-TOOL also enables the
54 simulation of ¹⁴C turnover. The simple model structure facilitates calibration and requires few
55 inputs (mean monthly air temperature, soil clay content, soil C/N ratio and C in organic inputs). The
56 model was parameterised using data from 19 treatments drawn from seven long-term field
57 experiments in the United Kingdom, Sweden and Denmark. It was found that the initial SOC
58 content had to be optimised for each experiment, but also that one set of values for other model
59 parameters could be applied at all sites. With this set of parameters, C-TOOL can be applied more
60 widely to evaluate effects of management options on SOC storage in temperate agricultural soils. C-
61 TOOL simulates observed losses of SOC in soils under intensive agricultural use and the gain in
62 SOC derived from large inputs of animal manure and inclusion of perennial grassland. The model
63 simulates changes in SOC for the entire profile, but lack of data on subsoil SOC storage hampers a
64 proper model evaluation. Experimental verification of management effects on subsoil C storage,
65 subsoil C inputs from roots, and vertical transport of C in the soil profile remains prioritised
66 research areas.

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69 **Key words:** Soil carbon storage, modelling, C-TOOL, agriculture, management, mineral soils

70

71 **1. Introduction**

72 Soil organic carbon (SOC) in the form of organic matter not only contributes to soil quality, it also
73 accounts for about twice as much as the carbon (C) found as CO₂ in the atmosphere (Lal, 2004).
74 Major uncertainties in the global C budget are associated with changes in SOC stored in agricultural
75 soils (Stockmann et al., 2013). Losses of SOC from previous and current soil management remain
76 an important source of atmospheric CO₂, with SOC stocks continuing to decline for decades to
77 centuries after the start of cultivation (Johnston et al., 2009). A number of abiotic factors exert an
78 overall control of SOC in long-term agricultural soils, but for a given soil within a given climate,
79 changes in SOC storage are determined by land use and management. Since changes in SOC
80 contents occur slowly and against a large background of C already present in the soil, repeated soil
81 sampling over decades is needed to experimentally verify effects of specific changes in land use and
82 soil management (Saby et al., 2008; Smith, 2004). Estimates of overall changes in SOC storage
83 have been based on regional inventories (Capriel, 2013; Chapman et al., 2013; Heikkinen et al.,
84 2013; Meersmans et al., 2009), simulation models (Andrén et al., 2008; Kirk and Bellamy, 2010;
85 van Wesemael et al., 2010; Webb et al., 2003) and on data from long-term field experiments
86 (Kätterer and Andrén, 1999; Powlson et al., 2011; Smith et al., 1997).

87 Reliable projections of changes in SOC at farm- and regional-scales are required to predict the
88 impact of agricultural activity on the global C cycle, to estimate the responses of climate changes
89 and to allow farmers and policy makers to develop and implement management options that may
90 reduce CO₂ emissions from agricultural soils and protect the soil resource. Dynamic process-
91 oriented simulation models are generally considered to be efficient tools for projecting the effects of
92 management on SOC and several models are able to simulate C turnover in agricultural soils. Some
93 are dedicated C models (e.g. RothC, ICBM, and Yasso07 (Andrén and Kätterer, 1997; Coleman and
94 Jenkinson, 1996; Tuomi et al., 2009)), while other models include nitrogen (N) and water, or have a

95 scope that extends to the ecosystem level (e.g. DNDC, CENTURY and Daisy (Hansen et al., 1991;
96 Li, 1996; Parton et al., 1987)). Most contemporary models are heavily parameterised, require
97 extensive input data, and attempt to simulate both short-term and long-term dynamics of C in the
98 soil (Petersen et al., 2002). Further, many simulation models are difficult to calibrate because of the
99 issue of equifinality, meaning that different parameterisations provide similar fits to observed data
100 (Beven and Freer, 2001). To simulate changes in SOC at farm- and regional-scales, models should
101 require as few parameters as possible while still including the core mechanisms that regulate C
102 turnover at the relevant timescale.

103 The C-TOOL model was developed to enable simulations of the medium- to long-term
104 changes in SOC in temperate mineral soils under agricultural management, using fewer parameters
105 and input data than the dynamic process-oriented models currently available. The model structure
106 was inspired by the models presented by Petersen et al. (2002) and Saffih-Hdadia and Mary (2008),
107 and shares many principles with other SOC turnover models, including CENTURY (Parton et al.,
108 1987), CN-SIM (Petersen et al., 2005), Daisy (Hansen et al., 1991), ICBM (Andrén and Kätterer,
109 1997) and RothC (Coleman and Jenkinson, 1996). C-TOOL considers the inputs and turnover of C
110 associated with three SOC pools in the topsoil (0-25 cm) and three corresponding pools in the
111 subsoil (25-100 cm), the transport of SOC from topsoil to subsoil, and emissions of CO₂.
112 Simulation of ¹⁴C natural abundance is also facilitated. In this paper we report the parameterisation
113 of the model using data from 19 treatments drawn from seven long-term field experiments in the
114 United Kingdom, Sweden and Denmark.

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119 **2. Materials and Methods**

120 **2.1. C-TOOL structure**

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

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

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

142 The ROM pool contains C in organic matter that has been rendered biologically resistant by
143 physico-chemical mechanisms. In C-TOOL, the ROM pool is assumed to have a very slow
144 turnover. Most SOC turnover models include a compartment that is either considered biologically
145 inert or has a very slow turnover time (Falloon and Smith, 2000), and ROM turnover is considered
146 of little importance in simulations over one or two centuries (Andrén and Kätterer, 1997).
147 Radiocarbon dating suggests that the smallest possible size of the ROM pool corresponds to ca.
148 10% of the SOC in topsoil (assuming that ROM is of almost infinite age) while the upper limit for
149 ROM is ca. 50% of the SOC (Petersen et al., 2005). Using inverse modelling and data from six
150 long-term bare fallow experiments, Barré *et al.* (2010) found the stable C pool to account for ca. 25
151 % of the initial SOC content (Barré et al., 2010) . Analyses of soil buried beneath a Bronze Age
152 burial mound showed that ca. 30 % of the original SOC had survived 3300 years under aerobic
153 conditions (Thomsen et al., 2008a).

154

155 **2.2. Transformations**

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

164 Tillage is often assumed to enhance the turnover of SOC (Chatskikh et al., 2009), but a recent
165 meta-analysis suggests that tillage does not affect total SOC stock but merely its distribution in the

166 topsoil layers (Luo et al., 2010). Adopting the paradigm of simplicity, C-TOOL does not consider
167 the effects of soil tillage intensity.

168

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

170

$$171 \frac{dC_i}{dt} = -k_i C_i F_T(T)$$

172

Equation 1

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

175 The temperature coefficient is modified to obtain unity at 10°C in the following manner

176 (Kirschbaum, 1995):

$$177 F_T(T) = 7.24 \exp \left[-3.432 + 0.168T \left(1 - \frac{0.5T}{36.9} \right) \right] \quad \text{Equation 2}$$

178 where T is temperature ($^\circ\text{C}$).

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

181

$$182 T(z,t) = \bar{T} + A(0) \exp \left(-\frac{z}{D} \right) \sin \left(\omega t - \frac{z}{D} \right) \quad \text{Equation 3}$$

183

184

185 where \bar{T} is the average monthly air temperature ($^\circ\text{C}$), $A(0)$ is the amplitude in air temperature at the
186 soil surface on a monthly basis ($^\circ\text{C}$), D is the damping depth (m), and ω is angular frequency of the

187 harmonic oscillation in temperature, $2\pi/P$; P is period (the length of each cycle, or distance from
188 one peak to the next).

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

191 The clay content influences the humification coefficient (h), which is the proportion of C that is
192 partitioned to the HUM pool (Figure 1). The clay response function is from Coleman and Jenkinson
193 (1996):

194

$$195 \quad R = 1.67(1.85 + 1.6\exp(-7.86X)) \quad \text{Equation 4}$$

196

197 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})

198 The constant 1.67 is used to adjust to observed values of R for all soils (Coleman and Jenkinson,
199 1996).

200 The humification coefficient (h) is then calculated as:

201

$$202 \quad h = \frac{1}{R + 1}$$

203 Equation 5

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

206 The amount of SOC that is removed either by transport to the subsoil or emitted as CO_2 from
207 the HUM pool is calculated simultaneously after the decomposition process (Figure 1). The same
208 procedure is applied to the ROM pool.

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

$$215 \quad f(cn) = \min(56.2cn^{-1.69}, 1)$$

Equation 6

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

222 2.3. Vertical transport of SOC

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

231 2.4. Simulation of ^{14}C abundance

232 The abundance of ^{14}C is simulated by C-TOOL. Although long-term C turnover in soil involves
 233 some isotope discrimination (Christensen et al., 2011), this is disregarded in C-TOOL. Radiocarbon
 234 measurements (^{14}C) are presented as per cent modern C (pM) or as the difference in ^{14}C content
 235 relative to a defined standard ($\Delta^{14}\text{C}$) (Petersen et al., 2002).

236

237

$$pM = 100 \frac{\sum_{i=1}^n \lambda_i}{\sum_{i=1}^n C_i}$$

238 Equation 7

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

241

242

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

243 Equation 8

244 Figure 2 shows the historical atmospheric content of ^{14}C in the Northern Hemisphere. These
 245 were obtained from Coleman and Jenkinson (2008). Before 1860, C-TOOL assumes that the
 246 radiocarbon age of the plant material entering the soil each year is zero with values of 0 and 100 for
 247 $\Delta^{14}\text{C}$ and pM , respectively.

248 C-TOOL assumes the ^{14}C concentration in plant materials and animal manures, which enter the
 249 soil in a given year, to be the same as that in atmospheric CO_2 . The ^{14}C values are given in units of
 250 "absolute" per cent modern (Stuiver and Polach, 1977). Thus the ^{14}C content in the C input for a

251 given year is expressed as $pM/100$ or $(\Delta^{14}C+1000)/1000$, i.e. taking the value for 1859 as 1.

252

253 **2.5. Implementation**

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

261

262 **2.6. Long-term experiments and treatments**

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

270 **2.6.1. Askov, Denmark**

271 Askov Experimental Station is located at 55° 28' N and 09° 07' E with an annual precipitation of 862
272 mm and a mean annual temperature of 7.7°C. The soil is a coarse sandy loam. Data were retrieved
273 from four different experiments: The Askov Long-Term Experiments on Animal Manure and

274 Mineral Fertilisers (Askov-LTE; Christensen et al., 2006) initiated in 1894 at the Lermarken site
275 with four fields/blocks (B2, B3, B4 and B5), a bare-fallow (vegetation-free) experiment situated
276 next to the B3- and B4-fields (ASK-FL1-B3 and ASK-FL1-B4, respectively) and running from
277 1956 to 1985 (Christensen, 1990; Christensen and Johnston, 1997), a small-plot bare-fallow
278 experiment situated out-doors in concrete cylinders (ASK-FL2) and running from 1956 to 1986
279 (Christensen, 1988; Christensen and Johnston, 1997), and a field experiment with one- to six-years
280 old grass-only ley (ASK-GRASS) also located at the Lermarken site (Christensen et al., 2009). In
281 this experiment, plots with grass ley were established every year over a period of six years, the plots
282 not yet in grass being sown to spring cereals. After six years, all grass leys (now 1- to 6-years old)
283 were ploughed under and sown to spring cereals. Soil C was determined for individual leys when
284 these were established and again when they were terminated.

285 The Askov-LTE data were extracted from three treatments in the B3-field: one kept unfertilised
286 (ASK-UNF), one receiving mineral fertiliser (1 NPK) at a standard rate for the given crop (ASK-
287 1NPK), and one receiving animal manure (1 AM) with a similar content of main nutrients (ASK-
288 1AM). Radiocarbon data (pM) were extracted from same three treatments in the B2-field. This field
289 has a different initial SOC level than the B3-field (Bol et al., 2005; Petersen et al., 2005). All SOC
290 data refer to 0-20 cm soil depth and a dry bulk density of 1.55 g cm^{-3} was used throughout the
291 study.

292 **2.6.2. Rothamsted, United Kingdom**

293 Rothamsted Research is located at $51^{\circ}49' \text{ N}$, $0^{\circ}22' \text{ W}$ with an annual precipitation of 704 mm (1971-
294 2000 mean) and a mean annual temperature of 9.5°C . The soil is a silty clay loam. Data were
295 extracted from two long-term field experiments: The Broadbalk Winter Wheat experiment
296 (BROAD) initiated in 1843 and the Hoosfield Spring Barley experiment (HOOS) initiated in 1852.
297 Three treatments in the Broadbalk experiment were considered (all applied since 1843): An

298 unfertilised treatment (BROAD-UNF), a treatment receiving 144 kg N ha⁻¹ yr⁻¹ and standard rates
299 of other plant nutrients (BROAD-MIN) and a treatment supplied with farmyard manure at an annual
300 rate of 35 Mg ha⁻¹ (BROAD-FYM). Yields are taken from the ‘continuous wheat’ Section 1 of the
301 experiment, where winter wheat has been grown every year since 1843, except for occasional
302 fallow years. Between 1926 and 1966, this Section was fallowed approximately one year in five to
303 control weeds, and neither manure nor fertiliser was applied. Three treatments in the Hoosfield
304 experiment were included: An unfertilised treatment (HOOS-UNF), a treatment receiving farmyard
305 manure each year 1852 to 1871 at an annual rate of 35 Mg ha⁻¹ and no manure thereafter (HOOS-
306 FYM-UNF), and a treatment receiving farmyard manure at an annual rate of 35 Mg ha⁻¹ since 1852
307 (HOOS-FYM). In 1968 all Hoosfield treatments were subdivided into four plots to test different
308 rates of fertiliser N (0, 48, 96 and 144 kg N ha⁻¹ yr⁻¹ as calcium ammonium nitrate). These rates
309 change cyclically each year, so the mean N rate over each four year period is 72 kg N ha⁻¹ yr⁻¹. The
310 SOC was sampled to a depth of 23 cm at all Rothamsted treatments, and measured dry bulk
311 densities ranged from 1 to 1.27 g cm⁻³ for BROAD and HOOS treatments. The initial SOC values
312 (1843 for Broadbalk and 1852 for Hoosfield) have been estimated, and SOC in the FYM treatments
313 has been adjusted for changes in soil bulk density (Johnston et al, 2009; Powlson et al, 2012).
314 Broadbalk SOC data is shown for the ‘continuous wheat’ sections only. At Broadbalk, the subsoil
315 SOC was measured in BROAD-UNF and BROAD-FYM (down to 69 cm depth in 1893) and
316 BROAD-MIN (down to 91 cm depth in 1893 and 21-91 cm depth in 1999). In addition, dry bulk
317 densities were measured at different depths in the subsoil of Broadbalk treatments (Dyer, 1902).

318 **2.6.3. Ultuna, Sweden**

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

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

333

334 2.7. Climatic data

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

337

338 2.8. Model parameterisation

339 C-TOOL contains several parameters that need to be estimated before the model can be applied
340 (Figure 1). The initial SOC content for each experiment and the HUM decomposition rate were
341 optimised by minimising the squared difference between observed and simulated values (see
342 below). For simplicity, we assumed that the initial SOC to a depth of 1 meter was partitioned with
343 47% to the topsoil (0-25 cm) and 53% to the subsoil (25-100 cm) (Batjes, 1996).

344 The annual input of organic C to a soil arises from many sources, including aboveground crop
345 parts shed during the growth period, stubble left after harvesting, and root-derived C deposited

346 during and after the growth phase. The C input from aboveground crop residues can be determined
347 by inverse modelling, crop modelling (Bruun et al., 2003) or by allometric relationships between
348 yields and C input to the soil (Kätterer et al., 2011). The simplest approach is to use allometric
349 relationships and this was used for the C-TOOL simulations. Dry matter yields for cereals were
350 reported separately for grain and straw, whereas for other crops, only total above-ground mass was
351 reported. Even when straw is harvested, a substantial fraction of the plant biomass is returned
352 directly to the soil. In conventional farming, 50% of the C in total non-grain production may be
353 returned, partly because these fractions are scattered as small particles or left in stubble and thus not
354 removed after baling (Jørgensen et al., 2007). This was the case for Rothamsted treatments. For the
355 field experiments at Askov and Ultuna, it was estimated that a quantity corresponding to 10% and
356 5% of the reported total above-ground biomass was recycled, respectively. The value for Ultuna is
357 relatively small because at harvest, the aboveground biomass is cut close to the soil surface
358 (Kätterer et al., 2011).

359 The belowground C inputs include dead roots and rhizodeposition. Gerwitz and Page (1974)
360 assumed that root-derived C was the only input to soil below the plough layer (25 cm here) and that
361 this input could be described by an exponentially decreasing depth distribution. According to
362 Kätterer *et al.* (2011), 71% of the roots are allocated to the upper 20 cm, 80% to 30 cm and 85% to
363 40 cm. The fraction of the root-derived C allocated to the topsoil (0-25 cm) depends on crop type
364 and was fixed as 70% for autumn sown crops (Kätterer et al., 1993), 80% for spring sown crops
365 (Hansson and Andréén, 1999), and 90% for grassland (Kätterer and Andréén, 1999). Values for
366 carbon allocation to roots are crop specific and were derived from various studies (Table 2). The C
367 concentration in plant dry matter assumed to be 45% in all crop parts. Using the parameters in Table
368 2, Table 3 shows the allometric calculations of total C deposition.

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

378 Guenet *et al.* (2013) found that FOM decomposition rates may range from 0.2 to 10 yr^{-1} . In our
379 study, the decomposition rate of the FOM pool (k_{FOM} , 1.44 yr^{-1}) was taken from Petersen *et al.*
380 (2005). The initial fraction of SOC allocated to the topsoil ROM pool was 0.405 and the
381 decomposition rate of ROM pool (k_{ROM}) was set to $4.63 \times 10^{-4} yr^{-1}$ so that the simulated ^{14}C age of
382 Askov soils equals that of the “pre-bomb” measurements. The fraction of topsoil HUM partitioned
383 to the ROM pool (f_{ROM}) was set to 0.012, a value that under steady state conditions maintains the
384 fraction of SOC in the ROM pool at 0.405 (Petersen *et al.*, 2005).

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

392 The two remaining C-TOOL parameters; i.e. the decomposition rate of HUM (k_{HUM}) and the
393 total initial soil C content in the long-term treatments were estimated by simultaneous optimisation,
394 utilising a Marquard-Levenberg algorithm (Marquard, 1963). The optimisation was performed with
395 a weighted squared error sum as the target function, using measured topsoil SOC data and the
396 corresponding simulated data. The initial distribution of SOC between HUM and ROM pool
397 influences C-TOOL simulations (Bruun and Jensen, 2002), but this distribution cannot be related to
398 measurable entities. The procedure used when optimising the initial SOC content and k_{HUM} was to
399 begin the simulations with an initialisation period of 30 years i.e. prior to the period for which
400 measurements were available. For each treatment, the total SOC at the start of the initialisation
401 period was optimised on the measured value at the start of the experiment, with the condition that
402 the partitioning of SOC between pools was: FOM, 0; HUM, 0.595; and ROM, 0.405 (see above).
403 The first five years of management applied to treatments amended with mineral fertilisers was
404 repeated six times in the initialisation period. The exceptions were: 1) the ASK-GRASS treatment
405 where information on the management (spring cereals amended with mineral fertilisers and straw
406 removal) preceding the experimental treatment was available (Christensen et al. 2009), and 2) the
407 Broadbalk and Hoosfield experiments where the unfertilised wheat and spring barley and straw
408 removal were considered as the management in initialisation period. The weighted target function,
409 as well as the other procedures for optimisation, was taken from Petersen *et al.* (2005). The target
410 function T was calculated as:

411

$$412 \quad T = \sqrt{\frac{\sum_i^m \sum_j^{n_i} \sum_k^{l_{ij}} (O_{ijk} - S_{ijk})^2}{\sum_i^m \sum_j^{n_i} l_{ij} O_{j...}^2}} \quad n$$

Equation 9

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

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

423

424 **2.9. Statistical analysis**

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

431

$$432 \quad \text{MBE} = \frac{\sum_{i=1}^n (P_i - O_i)}{n}$$

433 Equation 10

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

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

439

$$440 \text{ RMSE} = \sqrt{\sum_{i=1}^n (P_i - O_i)^2 / n}$$

441

Equation 11

442

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

445

$$446 R^2 = \left(\frac{\sum_{i=1}^n (O_i - \bar{O})(P_i - \bar{P})}{\left(\sum_{i=1}^n (O_i - \bar{O})^2 \right)^{\frac{1}{2}} \left(\sum_{i=1}^n (P_i - \bar{P})^2 \right)^{\frac{1}{2}}} \right)^2 \times 100$$

Equation 12

447

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

449

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

454

EF

$$= \frac{\sum_{i=1}^n (O_i - \bar{O})^2 - \sum_{i=1}^n (P_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2}$$

Equation 13

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3. Results

472 The C-TOOL simulations for the Askov bare fallow and grassland treatments are shown in Figure 3

473 and the results from the Askov-LTE treatments in Figure 4. Table 5 shows the partitioning of SOC

474 among C-TOOL pools at onset and at the end of the simulated periods.

475 With the exception of the ASK-1AM and ASK-GRASS treatments, a loss of topsoil C was
476 simulated at Askov. The mean annual loss was 0.6 Mg C ha⁻¹ in bare fallow treatments (ASK-FL1-
477 B3, ASK-FL1-B4, and ASK-FL2) and 0.2 and 0.1 Mg C ha⁻¹ in ASK-UNF and ASK-1NPK
478 treatment, respectively. An annual increase of approximately 0.9 Mg C ha⁻¹ was simulated for
479 topsoil of the ASK-GRASS treatment. At Askov, the simulations of subsoil C showed a decrease in
480 bare fallow, ASK-UNF, ASK-1AM and ASK-1NPK (Table 5), while subsoil C increased 1 Mg C
481 ha⁻¹ yr⁻¹ in the ASK-GRASS treatment. The simulations for the ASK-1AM treatment showed no
482 change in topsoil C storage; however, simulated changes in topsoil C of ASK-1NPK and ASK-
483 1AM did not concur with measured values (Figure 4b and 4c).

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

493 The simulated topsoil C in the Rothamsted treatments is shown in Figure 5. At Broadbalk, the
494 model simulated a small loss of topsoil C in BROAD-UNF (0.1 Mg ha⁻¹ yr⁻¹) while measurements
495 show no change. The model simulated little change of topsoil SOC in BROAD-MIN and an
496 increase in BROAD-FYM of 1 Mg C ha⁻¹ yr⁻¹ during the first 20 yrs., and then around 0.2 Mg C
497 ha⁻¹ yr⁻¹ during 1863-2010. The simulated results are in agreement with previous measurements
498 (Powlson et al., 2012). In Hoosfield, the simulation for HOOS-UNF showed a decrease in topsoil C

499 (0.1 Mg ha⁻¹ yr⁻¹) during the simulated period. For HOOS-FYM, SOC increased by 0.2 Mg ha⁻¹ yr⁻¹
500 while the HOOS-FYM-UNF treatment lost topsoil C at a rate of 0.2 Mg C ha⁻¹ yr⁻¹, once FYM was
501 no longer applied. Simulations for subsoil C at Rothamsted showed a decrease in the BROAD-
502 UNF, HOOS-UNF and HOOS-FYM-UNF treatment whereas an increase in subsoil C was
503 simulated for BROAD-MIN, BROAD-FYM and HOOS-FYM (Table 5). The subsoil organic C
504 contents at different depths were measured in three treatments in Broadbalk in 1893 and also one
505 treatment and one depth in 1999. In 1893, the 23-69 cm layer of BROAD-UNF, BROAD-MIN and
506 BROAD- FYM contained 29, 30 and 35 Mg C ha⁻¹, respectively (after Dyer, 1902), while the 23-91
507 cm layer of BROAD-MIN contained 42 Mg C ha⁻¹ (Jenkinson et al., 2008) . The corresponding
508 simulated subsoil C storage was 36, 44 and 52 Mg C ha⁻¹ in 25-100 cm layer of BROAD-UNF,
509 BROAD-MIN and BROAD-FYM, respectively. In 1999, the measured subsoil C content in the 23-
510 91 cm layer of BROAD-MIN was 49 Mg C ha⁻¹ (Jenkinson et al., 2008) while C-TOOL simulated
511 54 Mg C ha⁻¹ in the 25-100 cm layer.

512 The C-flows simulated for 2010 by C-TOOL was compared for BROAD-UNF and BROAD-
513 FYM treatments. The simulated SOC pools and C flows for BROAD-UNF treatment were: 20 Mg
514 C ha⁻¹ in topsoil, 31 Mg C ha⁻¹ in subsoil, 1 Mg C ha⁻¹ yr⁻¹ emitted as CO₂ from topsoil and subsoil,
515 and 0.1 Mg C ha⁻¹ yr⁻¹ transported from topsoil to subsoil. The corresponding values for BROAD-
516 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.

517 C-TOOL simulations for topsoil C in 0-25 cm showed a good fit with measured data at Ultuna.
518 The treatments ULT-FL, ULT-UNF, ULT-MIN and ULT-STR showed losses of topsoil C
519 corresponding to 0.4, 0.3, 0.2 and 0.1 Mg C ha⁻¹ yr⁻¹, respectively (Figure 6). However, SOC
520 increased in topsoil of ULT-FYM (0.1 Mg C ha⁻¹ yr⁻¹). The simulation of SOC in the ULT-MIN-
521 STR treatment showed almost no change in topsoil C. In Ultuna, subsoil C decreased in ULT-FL,

522 ULT-UNF, ULT-MIN, ULT-FYM and ULT-STR during the simulation period; however, this was
523 not the case for ULT-MIN-STR treatment (Table 5).

524 Statistical analysis was performed not for individual treatments but for each site, whereby the
525 degrees of freedom and hence the robustness of the analysis were increased (Table 6). The MBE
526 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
527 ha⁻¹. Values for R² were equal to or above 90 for all three sites, indicating a satisfactory overall
528 agreement between simulated and measured values. The EF value was positive for all the
529 experimental sites.

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541 **4. Discussion**

542 **4.1. Topsoil C**

543 The C-TOOL estimates showed satisfactory fits to measured topsoil organic C in most of the
544 treatments considered in this study (Figure 3 to 6). The best fits were obtained for bare-fallow soil
545 (except ASK-FL2) and soil kept unfertilised (except BROAD-UNF). The major discrepancy

546 between measured and modelled topsoil C found for the bare-fallow treatment ASK-FL2 may be
547 ascribed to the set-up of this experiment. The ASK-FL2 was a small-plot experiment based on
548 topsoil that was retrieved from permanent grassland and coarsely sieved before being placed in the
549 cylinders (Christensen, 1988). This soil with a high initial content of labile SOC showed a steeper
550 decline in SOC than was modelled by C-TOOL. The more intense turnover of SOC could not
551 apparently be captured by C-TOOL with its present parameterisation, and the initialisation run did
552 not match the measured initial SOC storage in the pre-fallow grassland soil. In contrast, the two
553 field-based bare-fallow experiments ASK-FL1-B3 and ASK-FL1-B4 (Christensen, 1990) had a
554 long history of arable four-course rotations with removal of harvestable plant biomass and thus a
555 much smaller initial content of labile SOC.

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

567 Calculations of the cumulated input of C from the crop to the topsoil involved the use of
568 allometric functions. This approach has the advantage of simplicity and enables the model to be
569 used in situations where the only available crop data are crop types and yields of harvested biomass.

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

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

590

591 **4.2. Subsoil C**

592 It is well recognized that subsoils (30-100 cm) typically store about 50 % of the SOC found in the
593 0-100 cm soil profile (Batjes, 1996), but the impact of agricultural management is generally

594 considered to affect only SOC stored in the topsoil. However, accumulating evidence from
595 monitoring programs shows that agricultural management may have decadal scale impacts also on
596 SOC storage in subsoils (e.g. Taghizadeh-Toosi et al., 2014). While most simulation models do not
597 explicitly consider SOC turnover in subsoils, C-TOOL was developed to encompass the vertical
598 distribution of SOC down to 1 meter. In simulation models that explicitly include subsoil SOC (e.g.
599 RothPC-1; Jenkinson and Coleman, 2008), the basic mechanisms that regulate SOC turnover is
600 taken to be the same for topsoil and subsoil SOC pools. This is also true for C-TOOL. However,
601 there is accumulating evidence that the turnover of SOC in topsoil and subsoil is subject to different
602 regulatory mechanisms (Fontaine et al., 2007; Salomé et al., 2010), and that the vertical transport of
603 labile and stable SOC in the soil profile also differ (Braakhekke et al., 2013; Guenet et al., 2013).
604 Different processes such as leaching of dissolved and particulate organic matter, bioturbation as
605 well as stratified root inputs and differential C turnover may affect C contents down the soil profile
606 (Rumpel and Kögel-Knabner, 2011). It has been indicated that root litter is a dominant source of
607 subsoil SOC and also that roots may contribute more to refractory SOC pools than above-ground
608 residues (Kätterer et al., 2011).

609 In our study, C-TOOL was used to simulate SOC content down to 1 m depth, but C-TOOL was
610 optimised on the measured data for the topsoil only. Indeed, optimisation on the topsoil as well as
611 subsoil dataset may improve the prediction of SOC storage. The lack of experimental data on
612 changes in subsoil C storage obviously hampers a proper evaluation of the ability of C-TOOL to
613 simulate subsoil C turnover. The few data from the Broadbalk experiment are not sufficient. We
614 note, however, that the simulation of SOC in subsoil showed a decrease of SOC in the bare fallow
615 and unfertilised treatments while most of the manured, fertilised and grassland treatments showed
616 an increase in subsoil SOC storage. However, verification of management effects on subsoil C

617 storage, subsoil C inputs from roots, vertical transport of C in the soil profile, and verification of
618 different regulatory mechanisms for C turnover in subsoils should be given high priority.

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632 **Perspectives and Conclusions**

633 Compared to other SOC simulation models such as RothC, Daisy and CENTURY, C-TOOL
634 requires fewer parameters and inputs. In our study, the C-TOOL model efficiency was above 0.8 for
635 topsoil in all three sites. Farina *et al.* (2013) used RothC to simulate topsoil C storage for selected

636 treatments in the Rothamsted Broadbalk Continuous Wheat experiment and found a model
637 efficiency of 0.98. With C-TOOL we obtained a model efficiency of 0.83. However, the clay
638 response function in RothC and C-TOOL needs to be modified based on the results from a recent
639 meta-analysis study (Liu et al., 2014). Whether the trade-off between model efficiency and demand
640 for input data and parameterisation is acceptable will depend on the purpose of the simulations.
641 When the focus is to simulate farm- and regional-scale effects of management on medium to long
642 term storage of SOC in temperate well-drained mineral soils, we consider C-TOOL to be a valid
643 alternative to using a more complex model with default values for parameters, in situations where
644 these would be expected to vary among locations.

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

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

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945 axes.

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947 Hoosfield (d, e, and f) experiments in Rothamsted, United Kingdom

948 **Figure 6.** Measured and simulated SOC content at 0-25 cm depth in the different treatments at
949 Ultuna, Sweden

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

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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*	Cont. spring barley	1852- present
HOOS-FYM	Rothamsted, UK	9.2	704	23	Farmyard manure*	Cont. spring barley	1852- present
HOOS-FYM-UNF	Rothamsted, UK	9.2	704	23	Farmyard manure until 1871, then unfertilized*	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

952 * From 1968 all HOOS treatments received a mean N rate of 72 kg N ha⁻¹ yr⁻¹

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

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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

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

961 **Table 3.** Calculations of total C (Mg ha⁻¹) deposited in the top- and sub-soil

962

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 (0-25cm)

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_{below}) 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, $\varepsilon = 0.45$, $\xi = 0.7$ (winter crops), 0.8 (spring crops) or 0.9 (grassland).

964 **Table 4.** C-TOOL parameters and values

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C-TOOL Parameter	Value
Initial C content (Mg ha ⁻¹)	Optimised for each treatment
Initial f _{HUM} (Top & Sub soil)	0.595
Initial f _{ROM} (Top & 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*
k _{ROM} (yr ⁻¹)	4.63 × 10 ⁻⁴
t _F	0.03
f _{CO2}	0.628

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*Standard error

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982 **Table 5.** The size of C-TOOL simulated SOC pools (Mg C ha⁻¹) in the topsoil (0-25 cm) and
 983 subsoil (25-100 cm) at the first year of initialisation, onset and end of simulation runs of various
 984 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*	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

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

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992 **Table 6.** Values of MBE, RMSE (%), R² and EF for simulated and measured topsoil C of each
993 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

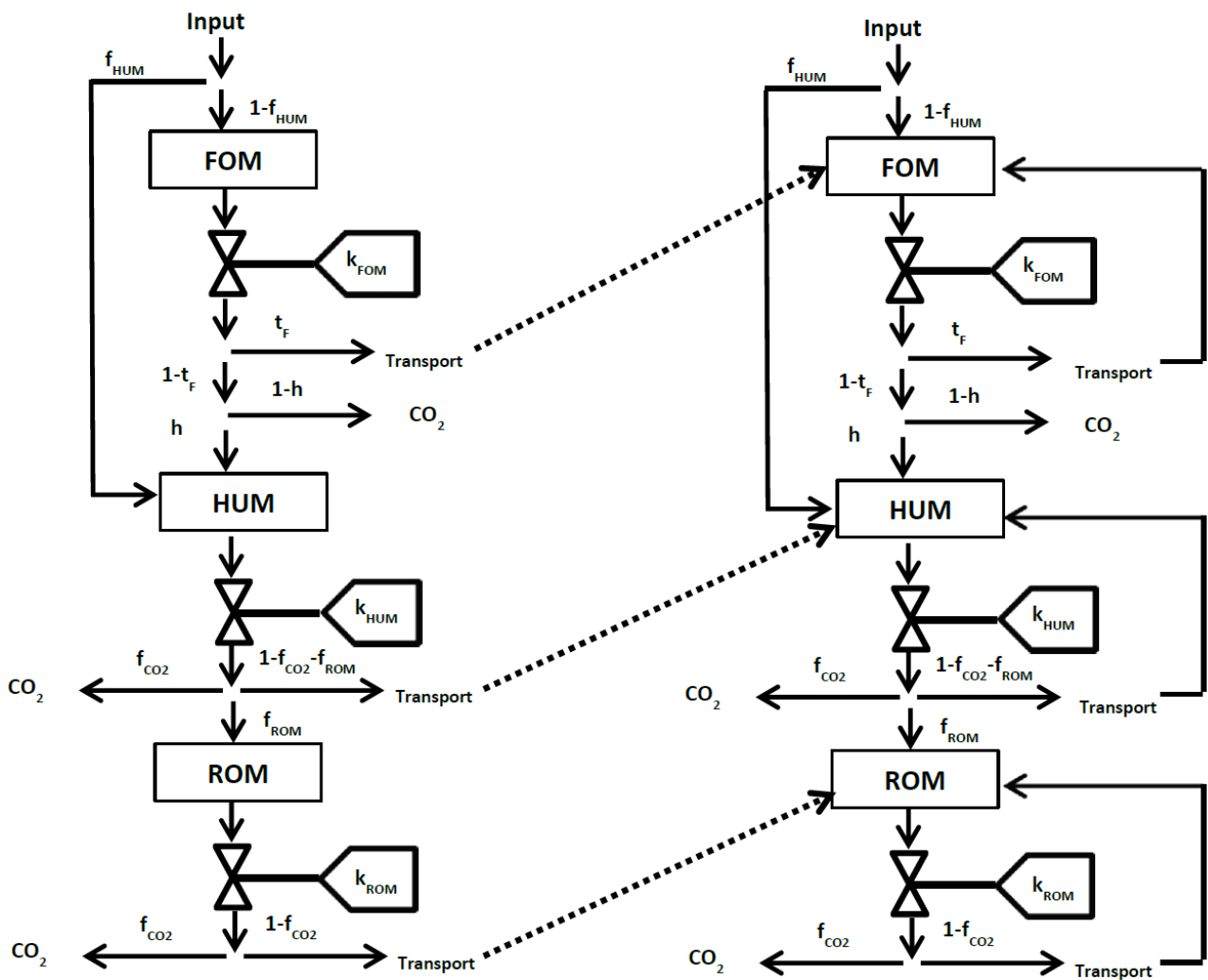
994 MBE: mean bias error; RMSE: root mean square error; R²: coefficient of determination; EF: model efficiency.
995 The number of observations were 146, 63 and 114 in Askov, Rothamsted and Ultuna; respectively.
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Figure 1. C-TOOL model structure for top and subsoil; FOM: Fresh Organic Matter, HUM:

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Humified Organic Matter, ROM: Resistant Organic Matter, f_{HUM} : fraction of input going

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to HUM (f_{HUM} is > 0 for manure and 0 for plant residues), k_{FOM} : decomposition rate of

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FOM, k_{HUM} : decomposition rate of HUM, f_{ROM} : fraction of FOM going to ROM, k_{ROM} :

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decomposition rate of ROM, t_F : The fraction going to downward transport, h :

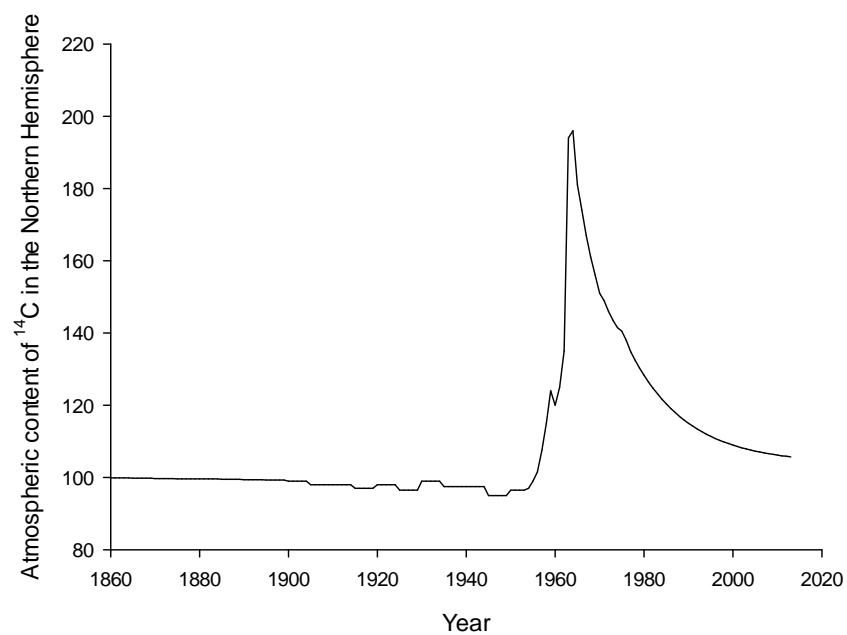
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Humification coefficient, f_{CO_2} : fraction of released CO_2 . NOTE The rate constants and

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fraction are the same for both topsoil and subsoil.

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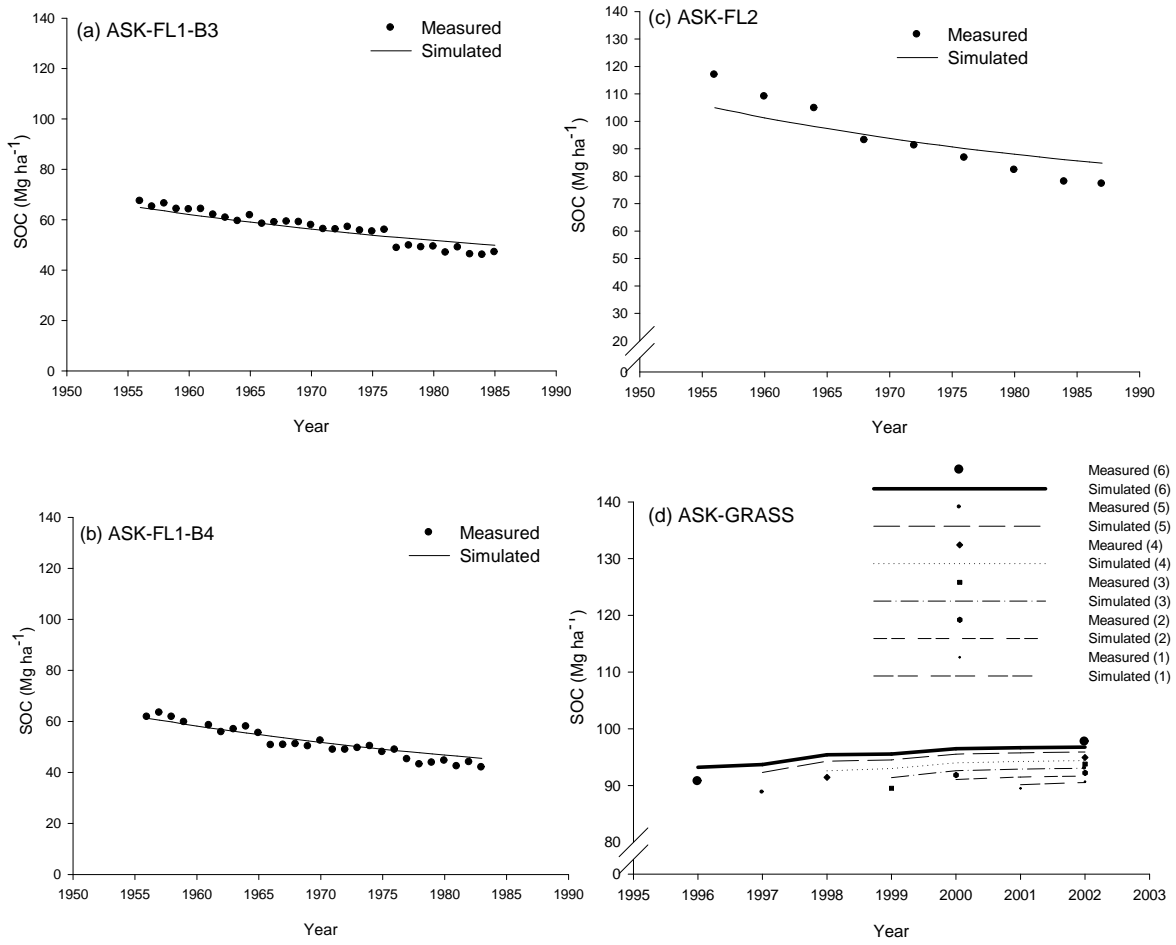
1012 **Figure 2.** Atmospheric content of ¹⁴C in the Northern Hemisphere, taken as 100 per cent modern C

1013 (*pM*) in 1859 (Coleman and Jenkinson, 2008)

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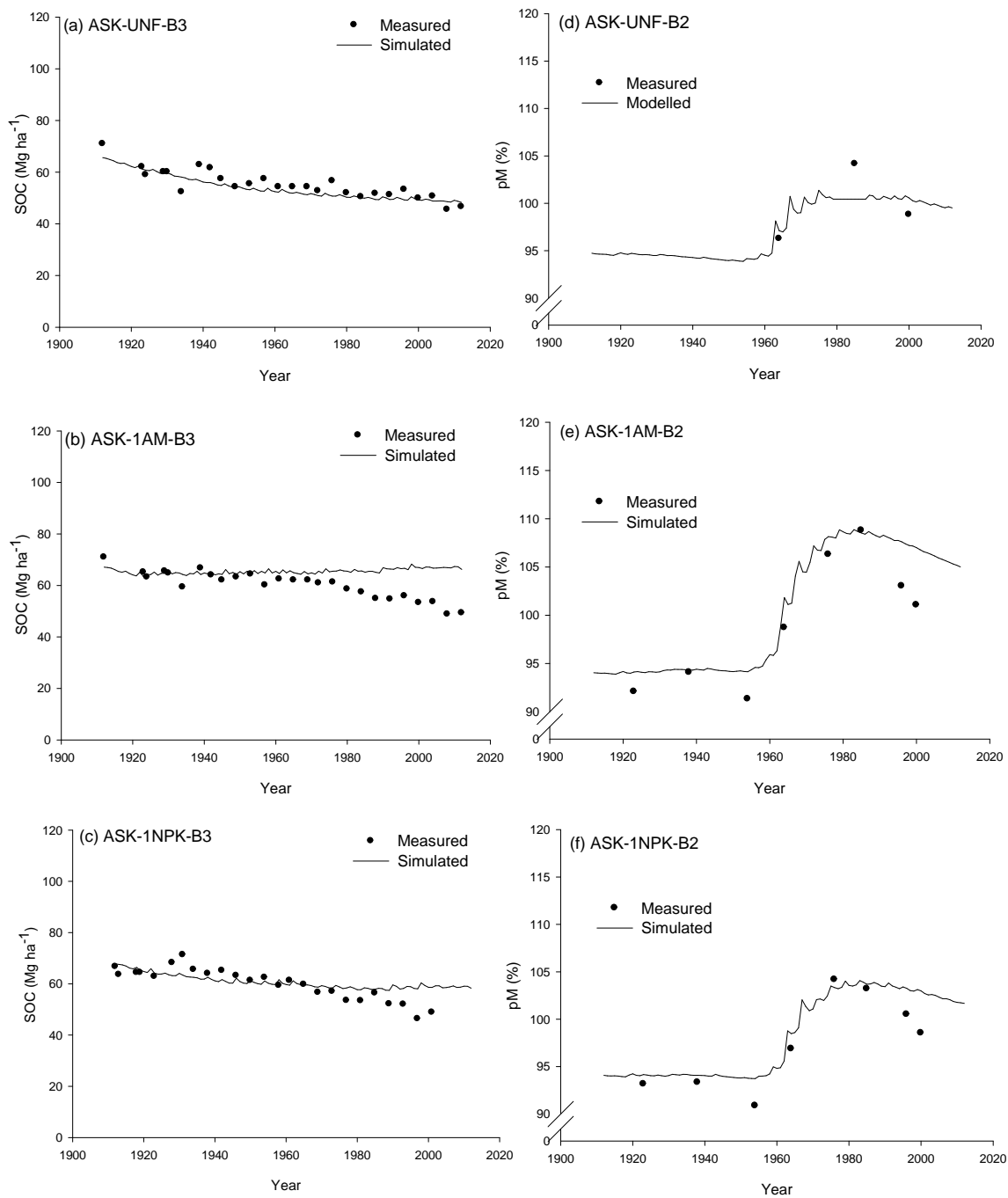
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1018 **Figure 3.** Measured and simulated SOC content at 0-25 cm depth in bare fallow (a, b, and c) and
 1019 grassland (d) treatments in Askov, Denmark. NOTE The numbers in parenthesis in (d)
 1020 show the age of grass leys (from 1 to 6 years). The thickest line and symbol
 1021 indicate the oldest grass ley.



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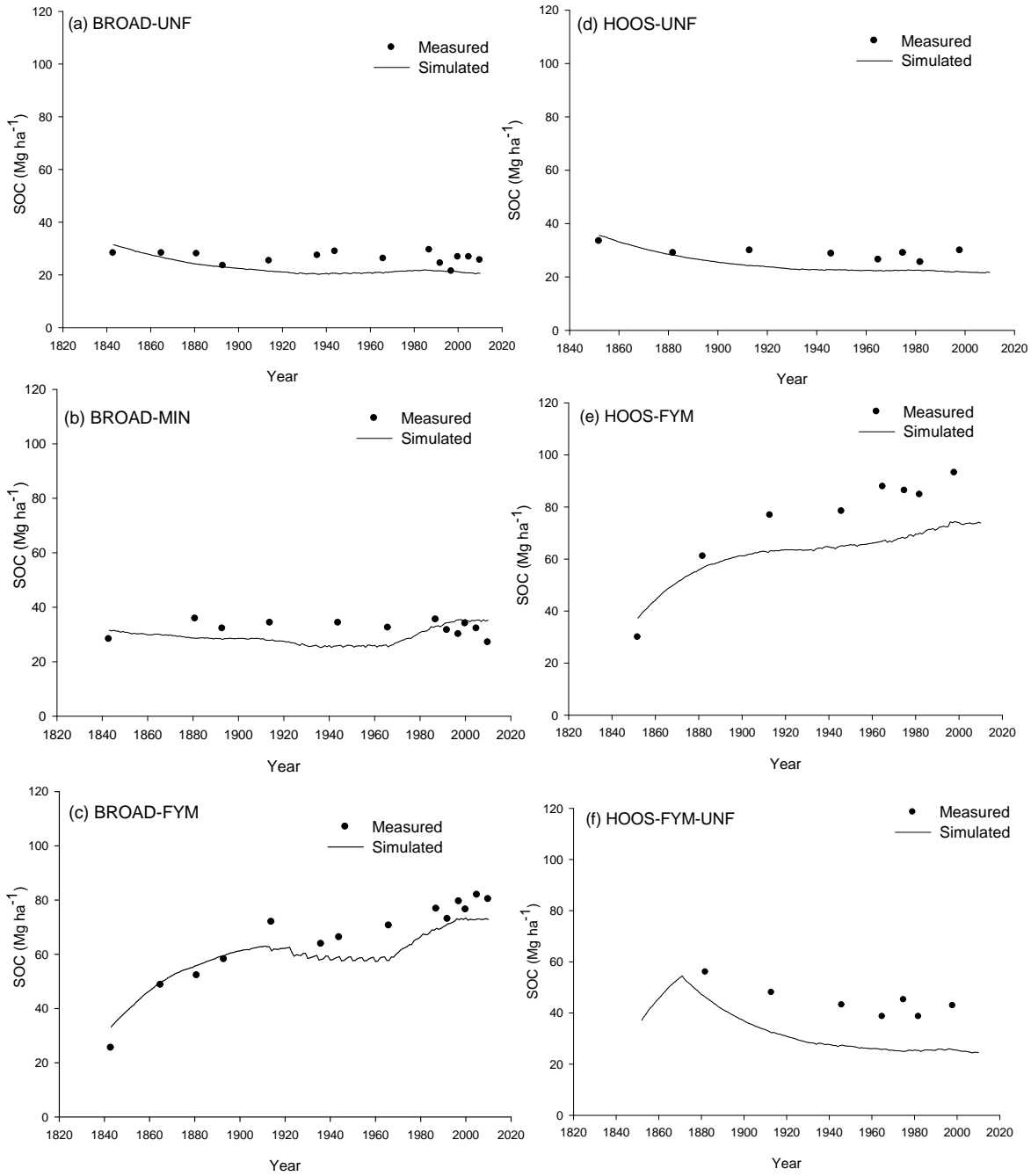
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Figure 4. Measured and simulated SOC content at 0-25 cm depth in different treatments of Askov B3-field crop rotations (a, b and c); Measured and simulated ^{14}C content at 0-25 cm depth in different treatments of Askov B2-field crop rotation (d, e, and f). NOTE the different units on y axes.

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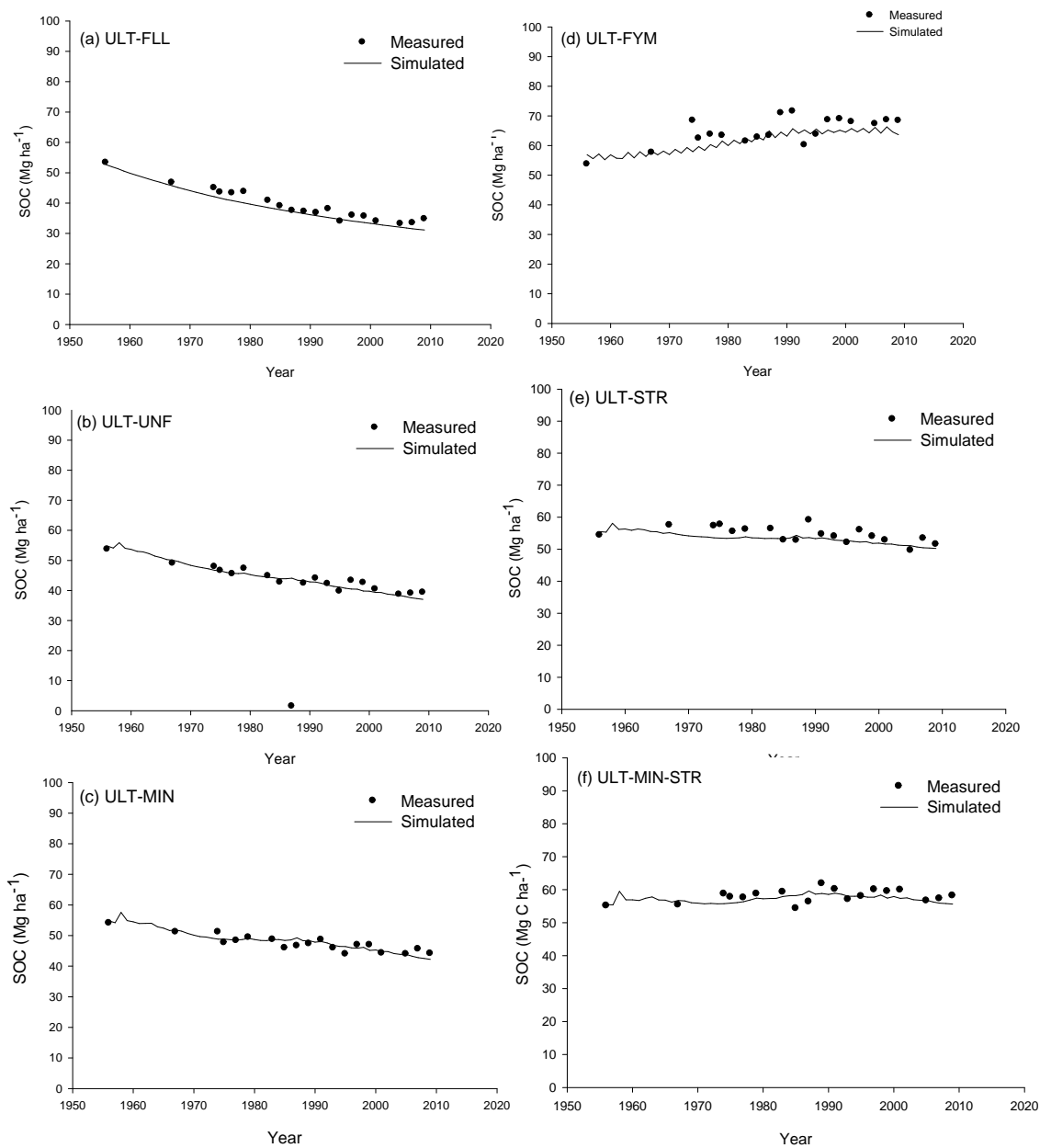
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1029 **Figure 5.** Measured and simulated simulated SOC content at 0-25 cm depth in Broadbalk (a, b, and

1030 c) and Hoosfield (d, e, and f) treatments in Rothamsted, United Kingdom

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1034 **Figure 6.** Measured and simulated SOC content at 0-25 cm depth in the different treatments at
 1035 Ultuna, Sweden