

Model to Estimate Carbon in Organic Soils – Sequestration and Emissions (ECOSSE).

User-Manual

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Table 1. Symbols used in equations

Symbol	Definition	Units
c_3	Constant used in calculating pH rate modifier for anaerobic decomposition	
c_4	Constant used in calculating pH rate modifier for anaerobic decomposition	
$C_{ao,1}$	Crop / plant type specific empirical parameter describing return to C to soil by plant	kg C ha ⁻¹
$C_{ao,2}$	Crop / plant type specific empirical parameter describing return to C to soil by plant	
$C_{ao,3}$	Crop / plant type specific empirical parameter describing return to C to soil by plant	
$C_{ao,4}$	Crop / plant type specific empirical parameter describing return to C to soil by plant	
$C_{ao,5}$	Crop / plant type specific empirical parameter describing return to C to soil by plant = 1	
C_{CH_4}	Production of methane	kg C ha ⁻¹ timestep ⁻¹ layer ⁻¹
C_{CO_2}	Production of methane	kg C ha ⁻¹ timestep ⁻¹ layer ⁻¹
$C_{CH_4 \rightarrow CO_2}$	Oxidation of methane to carbon dioxide	kg C ha ⁻¹ timestep ⁻¹ layer ⁻¹
C_{DOC}	Total DOC	kg C ha ⁻¹ yr ⁻¹ layer ⁻¹
$C_{DOC \rightarrow BIO}$	Decomposition of the DOC pool to produce BIO	kg C ha ⁻¹ timestep ⁻¹ layer ⁻¹
$C_{DOC \rightarrow CO_2}$	Decomposition of the DOC pool to produce CO ₂	kg C ha ⁻¹ timestep ⁻¹ layer ⁻¹
$C_{DOC,sol}$	DOC available in solution	kg C ha ⁻¹ yr ⁻¹ layer ⁻¹
C_{in}	Annual organic input to the soil	kg C ha ⁻¹ yr ⁻¹ layer ⁻¹
$C_{in,def}$	Default annual organic input to the soil	kg C ha ⁻¹ yr ⁻¹ layer ⁻¹
$C_{in,harv}$	C that is incorporated at harvest (e.g. stubble)	kg C ha ⁻¹
$C_{in,preharv}$	C that is incorporated before harvest	kg C ha ⁻¹
$C_{in,stubble}$	Amount of C in the stubble	kg C ha ⁻¹
$C_{in,straw}$	Amount of C in the straw	kg C ha ⁻¹
$c_{st,1}$	Empirical parameter describing C in stubble	
$c_{st,2}$	Empirical parameter describing C in stubble	
$c_{st,3}$	Empirical parameter describing C in stubble	
$c_{st,4}$	Empirical parameter describing C in stubble	
$c_{straw,1}$	Harvest index	
$c_{straw,2}$	Dry matter content of the straw	t dry matter / t straw

Symbol	Definition	Units
$c_{\text{straw},3}$	C : dry matter ratio of the straw	kg C / t straw dry matter
$c_{\text{straw},4}$	N : dry matter ratio of the straw	kg N / t straw dry matter
$C_{\text{in,tot}}$	Total annual organic inputs to the soil	kg C ha ⁻¹ yr ⁻¹
C_{IOM}	C in the IOM pool	kg C ha ⁻¹ layer ⁻¹
C_{R}	C in decomposing SOM pool, R	kg C ha ⁻¹ layer ⁻¹
$[C_{\text{R}}]$	Concentration of C in decomposing SOM pool, R	kg C ha ⁻¹ layer ⁻¹
$[C_{\text{R}}]_0$	Concentration of C in decomposing SOM pool, R, at start of the time step	kg C ha ⁻¹ layer ⁻¹
$[C_{\text{R}}]_t$	Concentration of C in decomposing SOM pool, R, at end of time step t	kg C ha ⁻¹ layer ⁻¹
$(C:N)_{\text{bac}}$	Typical C:N ratio of bacteria	
$(C:N)_{\text{fun}}$	Typical C:N ratio of fungi	
$(C:N)_{\text{LU}}$	C:N ratios for the different land uses	
$(C:N)_{\text{stable}}$	Stable C:N ratio of the SOM	
$C_{\text{tot,meas}}$	Measured total soil carbon	kg C ha ⁻¹ layer ⁻¹
$C_{\text{tot,sim}}$	Simulated total soil carbon	kg C ha ⁻¹ layer ⁻¹
γ	Soil dependent factor that accounts for different rates of CH ₄ diffusion and oxidation	
d	Depth of CH ₄ production	cm
d_{sink}	Depth at which soil becomes a net methane sink	cm
D_{ex}	Excess drainage when water flow is unrestricted compared to when water flow is restricted	mm layer ⁻¹
D_i	Unrestricted drainage from layer i	mm layer ⁻¹
D_{r}	Water drained with restriction to drainage	mm layer ⁻¹
D_{u}	Water drained with no restriction to drainage	mm layer ⁻¹
E	Decomposition efficiency	
f_{eff}	Fraction representing the efficiency of decomposition of DOC to BIO	
k_{BIO}	Rate constant for aerobic decomposition of BIO pool	time step ⁻¹
k'_{BIO}	Rate constant for anaerobic decomposition of BIO pool	time step ⁻¹
k_{DOC}	Rate constant for decomposition of DOC into BIO	time step ⁻¹
$k_{\text{C,in}}$	Rate constant for the incorporation of C in debris before harvest	
k_{DPM}	Rate constant for aerobic decomposition of DPM pool	time step ⁻¹
k'_{DPM}	Rate constant for anaerobic decomposition of DPM pool	time step ⁻¹

Symbol	Definition	Units
k_{HUM}	Rate constant for aerobic decomposition of HUM pool	time step ⁻¹
$k_{\text{N,in}}$	Rate constant for the incorporation of N in debris before harvest	
k'_{HUM}	Rate constant for anaerobic decomposition of HUM pool	time step ⁻¹
k_{R}	Rate constant for aerobic decomposition of SOM pool	time step ⁻¹
k'_{R}	Rate constant for anaerobic decomposition of SOM pool	time step ⁻¹
k''''_{R}	Rate constant for DOC production from SOM pool	time step ⁻¹
k_{RPM}	Rate constant for aerobic decomposition of RPM pool	time step ⁻¹
k'_{RPM}	Rate constant for anaerobic decomposition of RPM pool	time step ⁻¹
m'''_{b}	Denitrification rate modifier due to biological activity	
m_{c}	Aerobic decomposition rate modifier due to crop cover	
m'_{c}	Anaerobic decomposition rate modifier due to crop cover	
m''''_{c}	Rate modifier due to crop cover for production of DOC	
m''_{NH_4}	Nitrification rate modifier due to ammonium	
m'''_{NO_3}	Denitrification rate modifier due to nitrate	
m_{pH}	Aerobic decomposition rate modifier due to soil pH	
m'_{pH}	Anaerobic decomposition rate modifier due to soil pH	
m''_{pH}	Nitrification rate modifier due to soil pH	
m''''_{pH}	Rate modifier due to soil pH for production of DOC	
$m_{\text{pH,min}}$	Minimum value for aerobic decomposition rate modifier according to pH	
m_{t}	Aerobic decomposition rate modifier due to soil temperature	
m'_{t}	Anaerobic decomposition rate modifier due to soil temperature	
m''_{t}	Nitrification rate modifier due to soil temperature	
m''''_{t}	Rate modifier due to soil temperature for production of DOC	
m_{w}	Aerobic decomposition rate modifier due to soil moisture	
m'_{w}	Anaerobic decomposition rate modifier due to soil moisture	
m''_{w}	Nitrification rate modifier due to soil moisture	
m'''_{w}	Denitrification rate modifier due to soil moisture	
m''''_{w}	Rate modifier due to soil moisture for production of DOC	
m_{w0}	Aerobic decomposition rate modifier due to soil moisture at permanent wilting point	
m''_{w0}	Nitrification rate modifier due to soil moisture at	

Symbol	Definition	Units
	permanent wilting point	
ν	Soil factor accounting for diffusion and oxidation of methane	cm^{-1}
n	The number of the deepest layer in the soil profile	
N_d	Amount of nitrogen emitted from the soil during denitrification	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
N_{d,N_2}	Amount of N_2 gas lost by denitrification	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
N_{d,N_2O}	Amount of N_2O gas lost by denitrification	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
n_f	Proportion of N_2O produced due to partial nitrification at field capacity	
N_{fert}	Amount of fertiliser N applied	$\text{kg N ha}^{-1} \text{ timestep}^{-1}$
n_{gas}	Proportion of full nitrification lost as gas	
$N_{\text{in,harv}}$	N that is incorporated at harvest (e.g. stubble)	kg N ha^{-1}
$N_{\text{in,preharv}}$	N that is incorporated before harvest	kg N ha^{-1}
$N_{\text{in,tot}}$	Total annual organic inputs to the soil	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
$N_{\text{in,straw}}$	Nitrogen in straw	kg N ha^{-1}
N_n	The amount of N nitrified in the layer	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
N_{n,N_2O}	The amount of nitrified N emitted as N_2O in the layer	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
$N_{n,NO}$	The amount of nitrified N emitted as NO in the layer	$\text{kg N ha}^{-1} \text{ layer}^{-1} \text{ timestep}^{-1}$
N_{NH_4}	Concentration of ammonium in the soil	$\text{kg N ha}^{-1} \text{ layer}^{-1}$
n_{NO}	Proportion of full nitrification gaseous loss lost as NO	
N_{NO_3}	Concentration of nitrate in the soil	$\text{kg N ha}^{-1} \text{ layer}^{-1}$
$N_{\text{req,AG}}$	Total plant N requirement in above ground parts of the plant	$\text{kg N ha}^{-1} \text{ year}^{-1}$
$N_{\text{req,UG}}$	Total plant N requirement in below ground parts of the plant	$\text{kg N ha}^{-1} \text{ year}^{-1}$
$N_{\text{req,tot}}$	Total plant N requirement	$\text{kg N ha}^{-1} \text{ year}^{-1}$
$N_{v,\text{fym}}$	Ammonium lost by volatilisation from added manure	$\text{kg N ha}^{-1} \text{ timestep}^{-1}$
$p_{\text{as,fert}}$	Proportion of ammonium sulphate in the fertiliser	
p_{bac}	Proportion of bacteria in the soil	
$p_{\text{bac,min}}$	Minimum proportion of bacteria found in the soil	
$p_{\text{bac,max}}$	Maximum proportion of bacteria found in the soil	
p_{BIO}	Proportion of BIO produced on aerobic decomposition	$\text{kg C (kg C decomp.)}^{-1}$

Symbol	Definition	Units
p_{clay}	Proportion of clay in the soil	kg clay (kg soil) ⁻¹
p_{CO_2}	Proportion of CO ₂ produced on aerobic decomposition	kg C (kg C decomp.) ⁻¹
p_{fun}	Proportion of fungi in the soil	
pH	Soil pH	
pH''''_{max}	Critical threshold pH below which rate of DOC production starts to decrease	
pH_{max}	Critical threshold pH below which rate of aerobic decomposition starts to decrease	
pH_{min}	pH at which rate of aerobic decomposition is at minimum rate	
pH''''_{min}	pH at which rate of DOC production is at minimum rate	
pH_{opt}	Optimum soil pH for decomposition	
pH_{sens}	Sensitivity of the decomposition processes in this soil to pH	
p_{HUM}	Proportion of HUM produced on aerobic decomposition	kg C (kg C decomp.) ⁻¹
$p_{\text{in,AG}}$	Proportion of N in above ground crop that is incorporated in the soil	
$p_{\text{in,UG}}$	Proportion of N in below ground crop that is incorporated in the soil	
$p_{\text{N}_2,0}$	Proportion of nitrate N to total denitrification at which N ₂ emissions fall to zero	
$p_{\text{N}_2,f}$	Proportion of denitrified N lost as N ₂ at field capacity	
$p_{\text{NH}_4,\text{fym}}$	Proportion of ammonium in the manure	
p_{NO_3}	Proportions of denitrified gas emitted as N ₂ according to the nitrate content of the soil	
p_{r}	Proportion restriction in drainage at a particular site	
$p_{\text{urea,fert}}$	Proportion of urea in the fertiliser	
p_{w}	Proportion of denitrified gas emitted as N ₂ according to the water content of the soil	
ψ_{c}	Amount of water held in a particular soil layer above the permanent wilting point	mm layer ⁻¹
ψ_{i}	Amount of water held in a layer between field capacity and the soil at -100 kPa	mm layer ⁻¹
ψ_{f}	Amount of water held in a layer between field capacity and the permanent wilting point	mm layer ⁻¹
ψ_{s}	Amount of water held in a layer between saturation and the permanent wilting point	mm layer ⁻¹
Q_{10}	is a constant, describing the response of a process to temperature	
$Q_{\text{v,fym}}$	Volatilisation quotient for manure	
$Q_{\text{v,urea}}$	Volatilisation quotient for urea fertiliser	
$Q_{\text{v,as}}$	Volatilisation quotient for ammonium sulphate fertiliser	

Symbol	Definition	Units
R	Amount of rainfall	mm timestep ⁻¹
$R_{crit,v}$	Critical level of rainfall below which volatilisation starts.	mm timestep ⁻¹
t	Size of the time step	seconds
T_{air}	Mean air temperature for the period in the timestep	°C
T_{soil}	Mean soil temperature for the period in the timestep	°C
T_{sum}	Cumulative air temperature	°C days
τ	Methane transport factor	
u_1	Empirical parameter describing the sigmoid uptake of N by the crop	
u_2	Empirical parameter describing the sigmoid uptake of N by the crop	
$U_{r,1}$	Empirical parameter describing uptake of N in below ground parts of the plant	
$U_{r,2}$	Empirical parameter describing uptake of N in below ground parts of the plant	
$U_{r,3}$	Empirical parameter describing uptake of N in below ground parts of the plant	
$U_{t,1}$	Empirical parameter describing uptake of N in above ground parts of the plant	
$U_{t,2}$	Empirical parameter describing uptake of N in above ground parts of the plant	
$U_{t,3}$	Empirical parameter describing uptake of N in above ground parts of the plant	
w	Weeks till harvest	
W_{fym}	Fresh weight of manure added	t ha ⁻¹
W_{yield}	Crop Yield	t ha ⁻¹

PART A - MODEL DESCRIPTION

A1 Introduction

A1.1 Importance of long term estimates of aerobic decomposition

Climate change, caused by greenhouse gas (GHG) emissions, is one of the most serious threats facing our planet, and is of concern at both UK and devolved administration levels. Accurate predictions for the effects of changes in climate and land use on GHG emissions are vital for informing land use policy. Models that are currently used to predict differences in soil carbon (C) and nitrogen (N) caused by these changes, have been derived from those based on mineral soils or 'true' deep peat. It has been suggested that none of these models is entirely satisfactory for describing what happens to organic soils following land-use change.

Globally peatland covers approximately 4 million km², with a total C stock of ~450 Pg C in 2008 (Joosten, 2009). Peat is found across the planet with Russia, Canada, Indonesia and the United States having the largest peatland areas totalling just under 3 million km² (Joosten, 2009). Northern peatlands are the most important terrestrial C store. It is estimated that 20-30% of the global terrestrial C is held in 3% of its land area (Gorham, 1991). Over the Holocene, northern peatlands have accumulated C at a rate of 960 Mt C yr⁻¹ on average, making this ecosystem not only a substantial store of C, but also a large potential sink for atmospheric C (Gorham, 1991). Reports of Scottish GHG emissions have revealed that approximately 15% of Scotland's total emissions come from land use changes on Scotland's high C soils (Smith et al, 2007). It is therefore important to reduce the major uncertainty in assessing the C store and flux from land use change on organic soils, especially those which are too shallow to be true peats but still contain a potentially large reserve of C.

In order to predict the response of organic as well as mineral soils to external change we need models that more accurately reflect the conditions of these soils. Here we present a model for both organic and mineral soils that will help to provide more accurate values of net change to soil C and N in response to changes in land use and climate and may be used to inform reporting to GHG inventories. The main aim of the model described here is to simulate the impacts of land-use and climate change on GHG emissions from these types of soils, as well as mineral and peat soils. The model is a) driven by commonly available meteorological data and soil descriptions, b) able to predict the impacts of land-use change and climate change on C and N stores in organic and mineral soils, and c) able to function at national scale as well as field scale, so allowing results to be used to directly inform policy decisions.

A1.2 The ECOSSE approach

The ECOSSE model was developed to simulate highly organic soils from concepts originally derived for mineral soils in the RothC (Jenkinson and Rayner, 1977; Jenkinson et al. 1987; Coleman and Jenkinson, 1996) and SUNDIAL (Bradbury et al. 1993; Smith et al. 1996) models. Following these established models, ECOSSE uses a pool type approach, describing soil organic matter (SOM) as pools of inert organic matter, humus, biomass, resistant plant material and decomposable plant material (Fig 1a).

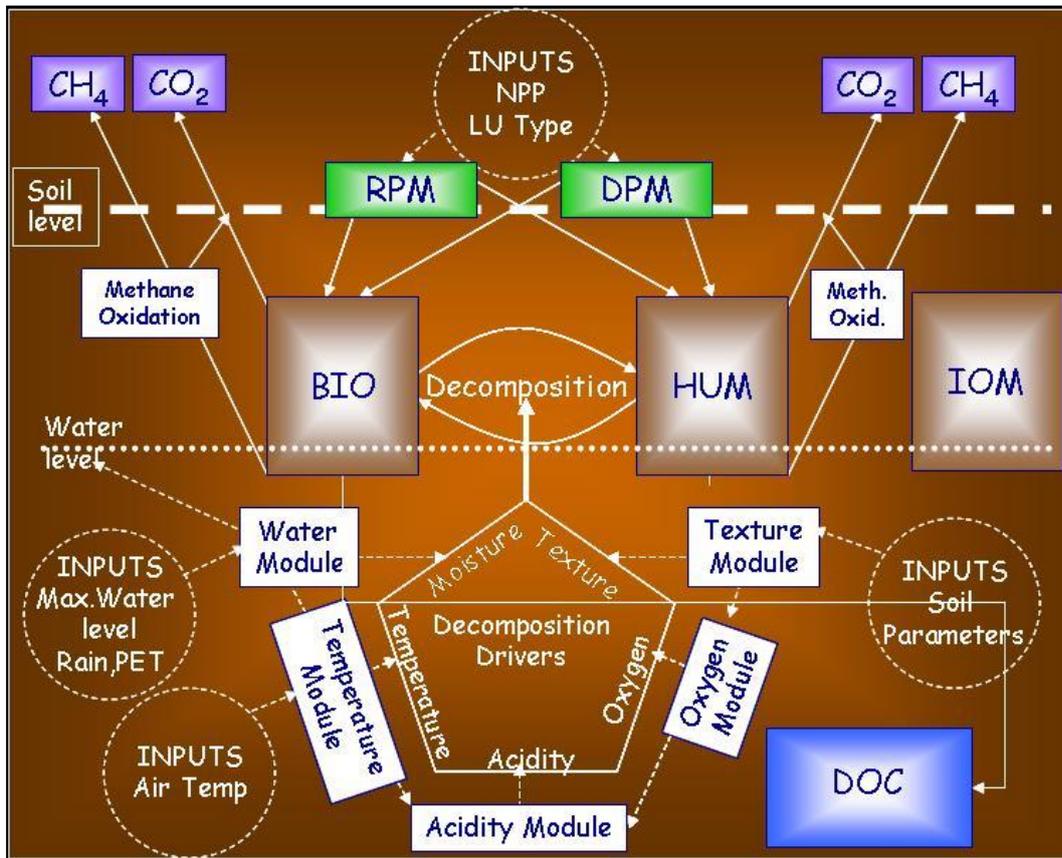
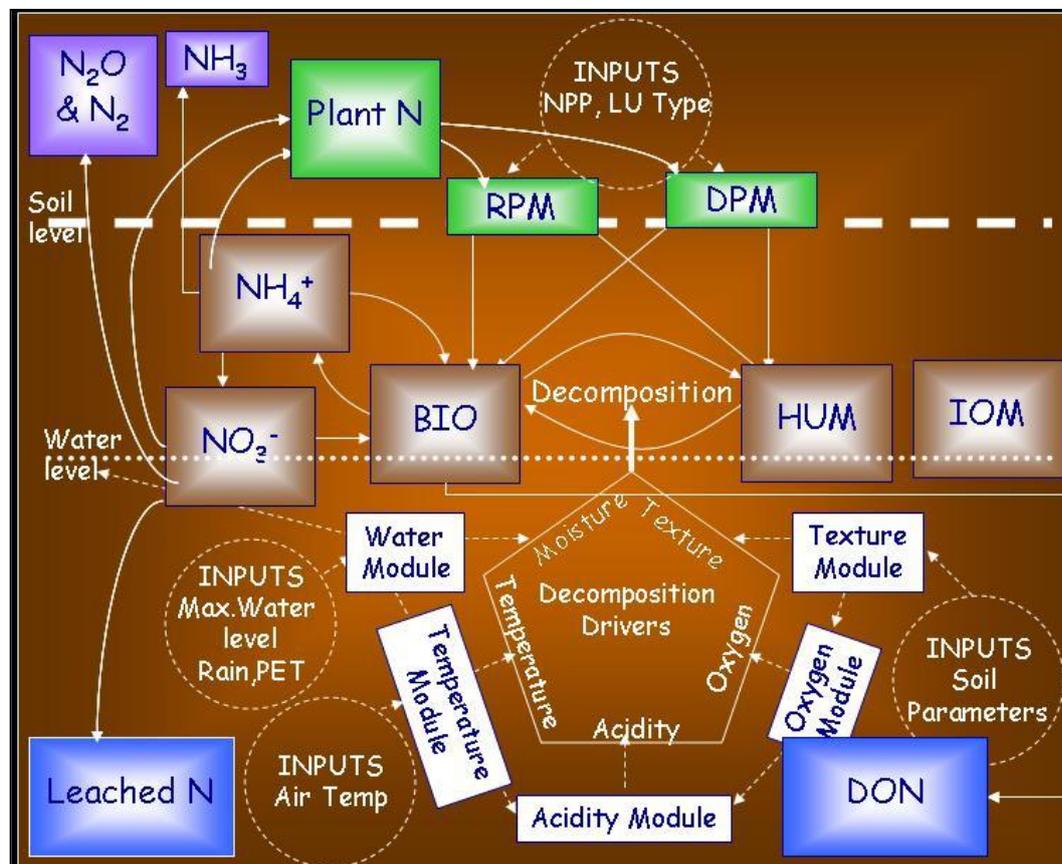


Figure 1a. Structure of the carbon components of ECOSSE



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Fig 1b. Structure of the nitrogen components of ECOSSE

All of the major processes of C and N turnover in the soil are included in the model, but each of the processes is simulated using only simple equations driven by readily available input variables, allowing it to be developed from a field based model to a national scale tool, without high loss of accuracy. ECOSSE differs from RothC and SUNDIAL in the addition of descriptions of a number of processes and impacts that are not important in the mineral arable soils that these models were originally developed for. More importantly, ECOSSE differs from RothC and SUNDIAL in the way that it makes full use of the limited information that is available to run models at national scale. In particular, measurements of soil C are used to interpolate the activity of the SOM and the plant inputs needed to achieve those measurements. Any data available describing soil water, plant inputs, nutrient applications and timing of management operations are used to drive the model and so better apportion the factors determining the interpolated activity of the SOM. However, if any of this information is missing, the model can still provide accurate simulations of SOM turnover, although the impact of changes in conditions will be estimated with less accuracy due to the reduced detail of the inputs. This novel approach will be discussed further below.

In summary, during the decomposition process, material is exchanged between the SOM pools according to first order rate equations, characterised by a specific rate constant for each pool, and modified according to rate modifiers dependent on the temperature, moisture, crop cover and pH of the soil. Under aerobic conditions, the decomposition process results in gaseous losses of carbon dioxide (CO_2); under anaerobic conditions losses as methane (CH_4) dominate. The N content of the soil follows the decomposition of the SOM (Fig 1b), with a stable C:N ratio defined for each pool at a given pH, and N being either mineralised or immobilised to maintain that ratio. Nitrogen released from decomposing SOM as ammonium (NH_4^+) or added to the soil may be nitrified to nitrate (NO_3^-). Carbon and N may be lost from the soil by the processes of leaching (NO_3^- , dissolved organic C (DOC), and dissolved organic N (DON)), denitrification, volatilisation or crop offtake, or C and N may be returned to the soil by plant inputs, inorganic fertilizers, atmospheric deposition or organic amendments. The soil is divided into 5cm layers, so as to facilitate the accurate simulation of these processes down the soil profile. The formulation and simulation approach used for each of these processes are described in detail below.

A2 The activity of soil organic matter decomposition

A2.1 Definition of pools used in ECOSSE

As already discussed, following the approach used in the RothC model (Coleman and Jenkinson, 1996), ECOSSE uses a pool type approach, describing SOM as pools of inert organic matter (IOM), humus (HUM), biomass (BIO), resistant plant material (RPM) and decomposable plant material (DPM) (Fig 1a). The IOM pool does not undergo decomposition; the C in this pool does not take part in soil processes either due to its inert chemical composition or its protected physical state. The HUM pool decomposes slowly, representing material that has undergone stabilization due to earlier decomposition processes. The BIO pool decomposes more rapidly and represents material that has undergone some decomposition but is still biologically active. The DPM and RPM pools are composed of undecomposed plant material, the DPM pool being readily decomposable while the RPM pool is more recalcitrant. The ratio of DPM to RPM defines the decomposability of the plant material that is added to the soil. Standard values for the ratio of DPM to RPM for the different land uses as used in

RothC are given in table 2, although these can be changed within ECOSSE for a specific instance of a land use type.

Table 2. The ratio of DPM to RPM for different land use types

Land use type	DPM:RPM ratio
Arable	1.44
Grassland (Improved grassland)	1.44
Forestry (Deciduous / Tropical woodland)	0.25
Semi-natural (Unimproved grassland / Scrub)	0.67

A2.2 Determining the initial sizes of soil organic matter pools

A2.2.1 Rapid determination of initial soil organic matter pool sizes

A method to determine the size of the SOM pools at the start of the simulation is provided by an equilibrium run of the RothC model. This rapid method used to calculate the size of SOM pools for the system at steady state given the inputs from plants and organic amendments is described in detail by Coleman and Jenkinson (1996). The relative proportions of the different SOM pools determines the activity of the SOM to decomposition; a higher proportion of a rapidly decomposing pool will result in a higher overall activity of the SOM, whereas a higher proportion of a slowly decomposing pool will result in a lower overall activity.

If plant inputs are well known and the soil has reached a steady state where no further increase or decrease in soil C is observed, the initial pool sizes can be determined directly from these specified inputs using the rapid method to calculate the SOM pools at the equilibrium steady state achieved using those plant inputs. In practice, however, the actual plant inputs to a system are rarely known with accuracy, even at field scale, because the full contribution of litter, debris and root exudates is very difficult to measure. As the model is scaled up for national simulations, it becomes even more difficult to accurately estimate the organic inputs to a system. Therefore, an iterative procedure is used to estimate the organic inputs from measured soil C.

An initial estimate of the total annual organic input is used to provide a first calculation of the C in each SOM pool at steady state. Added together with the amount of material in the IOM pool, the C in these pools provides an estimate of the total soil C simulated using the given organic inputs. An estimate for the amount of material in the IOM pool is given by Falloon et al. (1998),

$$C_{IOM} = 0.049 \times C_{tot,meas}^{1.139} \quad (1)$$

where C_{IOM} is the C in the IOM pool and $C_{tot,meas}$ is the measured total soil C, both given in $\text{kg C ha}^{-1} \text{ layer}^{-1}$. The total annual plant inputs are distributed according to the pattern of leaf fall and debris

inputs for the given land use type. Default values for the distribution of the plant inputs, shown in table 3, were obtained from the values provided by Falloon et al. (1998).

Table 3. The default distribution of plant inputs to the soil

Month	1	2	3	4	5	6	7	8	9	10	11	12
Arable												
0-30cm	0.00	0.00	0.30	0.30	0.30	0.60	1.87	0.00	0.00	0.00	0.00	0.00
30-100cm	0.00	0.00	0.30	0.30	0.30	0.30	1.17	0.00	0.00	0.00	0.00	0.00
> 100cm	0.00	0.00	0.30	0.30	0.30	0.30	1.17	0.00	0.00	0.00	0.00	0.00
Grassland (Improved grassland)												
0-30cm	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.89	0.25	0.25	0.25	0.25
30-100cm	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21
> 100cm	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21
Forestry (Deciduous / Tropical woodland)												
0-30cm	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24
30-100cm	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24
> 100cm	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24
Semi-natural (Unimproved grassland / Scrub)												
0-30cm	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48
30-100cm	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.00
> 100cm	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.00

The weather conditions are usually taken from a 30 year average of the long term weather data describing rainfall and air temperature at the site on a monthly time step. This underestimates the impact of weather conditions, as the extremes are smoothed out by the averaging process, but on a monthly time step, this has little impact on the simulations.

The precision of the value used as the initial estimate of total annual organic input is unimportant in this initial phase of the simulation because the model adjusts the organic inputs according to the ratio of simulated to measured soil C,

$$C_{in} = C_{in,def} \times \frac{C_{tot,meas}}{C_{tot,sim}} \quad (2)$$

where C_{in} is the actual annual organic input, $C_{in,def}$ is the default annual organic input, $C_{tot,meas}$ is the measured total soil C, and $C_{tot,sim}$ is the simulated total soil C, all given in $\text{kg C ha}^{-1} \text{ layer}^{-1}$. This equation provides a revised estimate of the total annual organic inputs, which is then used to rerun

the model to obtain a new simulation of the SOM pool sizes at steady state. Because the model is not linear, a few iterations of the above calculation are usually required before the simulated total soil C matches the measured value. When the simulated and measured values are within $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1}$, the SOM pool sizes and calculated plant inputs are used to represent the pools and inputs needed to achieve the observed soil C at steady state. Because the SOM pools have different rate constants, the relative proportions of these pools define the activity of the SOM turnover. The model may then be run forward, applying changes in the soil conditions, land use and climate to calculate their impact on the rate of aerobic SOM turnover.

The RothC equilibrium run is a useful approach, especially in national simulations, as it provides a very quick estimate of the rate of decomposition using very little input data. Any factors that are not explicitly described in the measurements used to drive the model will be subsumed into the description of the rate of decomposition provided by the relative pool sizes. For instance, if the soil is saturated for much of the year, this is reflected in a slower rate of decomposition, resulting in a higher observed total soil C, which then requires a larger component of the SOM to be composed of the more slowly decomposing HUM pool. If the saturated condition of the soil had been explicitly included in the measurements used to drive the model, the slowed rate of decomposition would instead have been described by a slowed decomposition rate under anaerobic conditions. This would have provided a more accurate simulation of the impact of any factors that might change the water table depth (such as changes in rainfall patterns). If the simulations are instead focusing on the impact on SOM turnover of changes in climate in soils that are likely to become saturated, it is important that the water table depth be included as an input driver, but if the soils are not likely to become saturated, this is less important. The user should be aware of any limitations in the results introduced by using less data to drive the model, but the ability to run simulations in this way, using only the data that are readily available, is a major advantage, especially in national simulations.

One deficiency in the approach described above is that the RothC equilibrium run includes no limitation in the rate of decomposition due to N availability. In many cases, N can significantly limit the rate of SOM turnover, and if the N limitation is not included in the model initializations, an underestimate of the rate of aerobic SOM turnover when N is non-limiting can result. If the N limitation is then applied, in the full ECOSSE simulation, the rate of decomposition will be slower than observed, as it is being slowed by N limitation as well as by the initialization of the SOM pools. As a result, SOM will start to accumulate rather than being at steady state when N limitation is included in the full ECOSSE simulation. If N limitation is likely to be a significant factor, a more time-consuming initialization procedure using the full ECOSSE simulation during the initialization is required.

A2.2.2 Initialization by full ECOSSE simulation

Because the full ECOSSE simulation includes a number of highly non-linear processes, the rapid method used in the RothC equilibrium run cannot be applied to ECOSSE. Therefore, initialization of the SOM pools using the full ECOSSE simulation requires the model to be run until the system reaches steady state. This can require the simulation to be continued for a number of years, and so can significantly increase simulation time. However, the approach has the advantage of taking full account of all processes included in ECOSSE, and allows the steady state conditions of the system to be specified in more detail. The mode of simulation differs, depending on the nature of the steady state.

Site at equilibrium

A site is considered to be at equilibrium if the total C content of soil has reached a steady state where the total organic inputs to the system are balanced by the total losses of soil C, and so the soil C content does not change significantly over the years. To initialize the model to an equilibrium steady state, the simulations are started with zero SOM in all pools. The organic inputs calculated by the RothC equilibrium run are added to the soil as specified by the distribution of plant inputs and organic amendments (table 3), and the weather conditions are taken from a 30 year average of the long term weather data describing rainfall and air temperature at the site on a monthly time step. The simulation is continued until the total soil C in the layer differs from the value at the same time in the previous year by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1}$. At this point, the spin-up is stopped, and the organic inputs adjusted as shown in equation (2). The spin-up is then rerun using the revised organic inputs. This iterative procedure is continued until the simulated soil C differs from the measured soil C by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1}$.

Site accumulating carbon at a constant rate

A site that is accumulating soil C is considered to be at steady state if the soil accumulates C at a constant rate that does not change significantly over the years. To initialize the model to an accumulating steady state, the simulations are again started with zero SOM in all pools and the organic inputs added each year as estimated by the RothC equilibrium run. In this case, the rate of change in soil C is calculated each year, and when the rate of change differs from the measured rate of C accumulation by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1} \text{ yr}^{-1}$, the spin-up is stopped. The organic inputs are adjusted as shown in equation (2), and the spin-up is rerun with the revised organic inputs. The iterative procedure is continued until the simulated soil C differs from the measured soil C by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1}$, so achieving simulations which match both the measured rate of C accumulation and the measured soil C content.

Site losing carbon at a constant rate

A degrading site is considered to be at a steady state if it is losing soil C at a constant rate that does not change significantly over the years. To initialize the model to a degrading steady state, the simulations are started using C in the SOM pools 10% higher than estimated by the RothC equilibrium run. The organic inputs estimated by the RothC equilibrium run are added each year and the annual change in soil C calculated. The soil C is allowed to run-down until the rate of change of soil C differs from the measured rate of C loss by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1} \text{ yr}^{-1}$. If the rate of C loss is always less than observed, the simulations are restarted using a higher increase in the SOM pools estimated by RothC. The organic inputs are adjusted as shown in equation (2), and the initialization rerun with the revised organic inputs. This iterative procedure is continued until the simulated soil C differs from the measured soil C by less than $0.0001 \text{ kg C ha}^{-1} \text{ layer}^{-1}$, so achieving simulations which match both the measured rate of C loss and the measured soil C content.

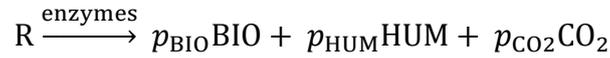
A2.3 Evaluation of the methods used to determine the initial sizes of the soil organic matter pools

An evaluation of the methods used to determine the initial sizes of the soil organic matter pools has been completed for a range of soil conditions, in a number of different soil environments and under different land uses. This work is currently being prepared for publication and so cannot be included

here. When published, a summary of the evaluation and a reference to the published paper will be provided.

A3 Aerobic decomposition of soil organic matter pools

Each pool is assumed to behave as a homogeneous unit, decomposing under aerobic conditions to produce carbon dioxide (CO₂), and pass a proportion of the C into the HUM and BIO pools.



where R is C in the DPM, RPM, BIO or HUM pool; and p_{BIO} , p_{HUM} and p_{CO_2} are the proportions of BIO, HUM and CO₂ produced on aerobic decomposition (kg C (kg C decomp.)⁻¹).

Using the definitions from RothC, the proportions p_{BIO} , p_{HUM} and p_{CO_2} are defined by the following relationships:

$$\frac{p_{\text{BIO}}}{p_{\text{HUM}}} = 0.85 \quad (3)$$

and

$$E = \frac{(p_{\text{BIO}} + p_{\text{HUM}})}{p_{\text{CO}_2}} = \frac{1}{1.67 \left(1.85 + 1.60 \exp(-7.86 \times p_{\text{clay}}) \right)} \quad (4)$$

where E is known as the decomposition efficiency, and p_{clay} is the proportion of clay in the soil (kg clay (kg soil)⁻¹). This rearranges to give

$$p_{\text{CO}_2} = 1 - E \quad (5)$$

$$p_{\text{HUM}} = \frac{0.85}{(1 + E)} \quad (6)$$

and

$$p_{\text{BIO}} = E - \frac{0.85}{(1 + E)} \quad (7)$$

It is assumed that the enzymes are in excess, so the rate of aerobic decomposition is only dependent on the concentration of C in the decomposing SOM pool, $[C_R]$ (kg C ha⁻¹), and can be assumed to be a first order reaction,

$$\frac{-dC_R}{dt} = k_R [C_R] \quad (8)$$

where k_R is the rate constant for aerobic decomposition of pool R (time step⁻¹); the rate constants used are as given in RothC; for DPM $k_{DPM} = 10 \text{ yr}^{-1}$, for RPM $k_{RPM} = 0.3 \text{ yr}^{-1}$, for BIO $k_{BIO} = 0.66 \text{ yr}^{-1}$, and for HUM $k_{HUM} = 0.02 \text{ yr}^{-1}$. This integrates to give the concentration of R at any time t after the start time,

$$[C_R]_t = [C_R]_0 (1 - \exp(-k_R t)) \quad (9)$$

where $[C_R]_t$ is the concentration of C in pool R at time t , and $[C_R]_0$ is the concentration of C in pool R at the start of the time step. Because the soil is not a clean system under constant environmental conditions, the rate equation must be modified to account for changes in the environment:

$$[C_R]_t = [C_R]_0 \left(1 - \exp(-k_R t \times m_w \times m_t \times m_c \times m_{pH}) \right) \quad (10)$$

where m_w , m_t , m_c and m_{pH} are rate modifiers that account for the impact of changes in soil moisture, temperature, crop cover and pH respectively. The form of these rate modifiers is described in the following sections.

A3.1 Impact of soil water on aerobic decomposition

The aerobic decomposition rate modifier due to soil moisture is expressed according to the volumetric water content, permanent wilting point, field capacity and saturated water content of the soil. The permanent wilting point is the limit below which plants can extract no more water from the soil, and it is assumed here that the micro-organisms in the soil will also be unable to access water below this level. Field capacity is the maximum water that the soil can hold against gravity, and therefore the maximum soil water content that can occur in a freely drained soil. Field capacity is generally assumed to be the optimum water content for aerobic decomposition because both water and oxygen are easily available. Below field capacity, water may be limiting; above field capacity, oxygen may be limiting. This can lead to a reduction in the rate of aerobic decomposition. As agricultural soils are usually freely drained, agricultural models often ignore water contents above field capacity, but because ECOSSE is designed for use across a range of land uses, water contents are included up to saturation.

Below field capacity, the rate modifier follows the equation derived for the SUNDIAL model (Bradbury et al. 1993), which assumes aerobic decomposition proceeds at its maximum rate as the soil dries from field capacity to the amount of water held at -100 kPa, but then decomposition is inhibited below -100 kPa until the soil is at its permanent wilting point:

$$m_w = 1 - \frac{((1 - m_{w0}) \times (\psi_f - \psi_c - \psi_i))}{\psi_f - \psi_i} ; \text{ (if } (\psi_f - \psi_c) > \psi_i, m_w = 1) \quad (11)$$

where m_{w0} is the rate modifier at permanent wilting point, ψ_c is the amount of water held in a particular soil layer above the permanent wilting point (mm layer⁻¹), ψ_i is the amount of water held between field capacity and -100 kPa (mm layer⁻¹), and ψ_f is the amount of water held between field capacity and the permanent wilting point (mm layer⁻¹). Bradbury et al. (1993) used measurements of the effects on N mineralisation made by Stanford and Epstein (1974) to set the rate modifier at the permanent wilting point to 60% of the maximum rate, ie. $m_{w0} = 0.6$. However, SUNDIAL was originally developed for use in UK soils, where soil drying is limited. By contrast, RothC, which has been applied globally, reduces the rate of decomposition to 20% of the maximum rate, ie. $m_{w0} = 0.2$, at the permanent wilting the point. Because ECOSSE is required to function in dry conditions as well as very wet conditions, the RothC minimum rate of $m_{w0} = 0.2$ is used in ECOSSE.

Similarly, above field capacity, the rate modifier is assumed to follow a linear decline to the minimum rate of 20%, ie. $m_{w0} = 0.2$, at saturation.

$$m_w = 1 - \frac{((1 - m_{w0}) \times (\psi_c - \psi_f))}{\psi_s - \psi_f} \quad (12)$$

where ψ_s is the water content between saturation and permanent wilting point. A linear decline is used because there is insufficient evidence to suggest a more refined relationship; in the absence of data suggesting a significant improvement can be achieved by using a more complex equation, the simplest form should be used to maintain model parsimony. The minimum rate of $m_{w0} = 0.2$ at saturation was obtained by fitting to incubation experiments where the rate of decomposition was measured in rice straw in soils with increasing water content up to saturation (Devevre and Horwarth, 2000). The form of the soil moisture rate modifier for aerobic decomposition is shown in Fig. 2.

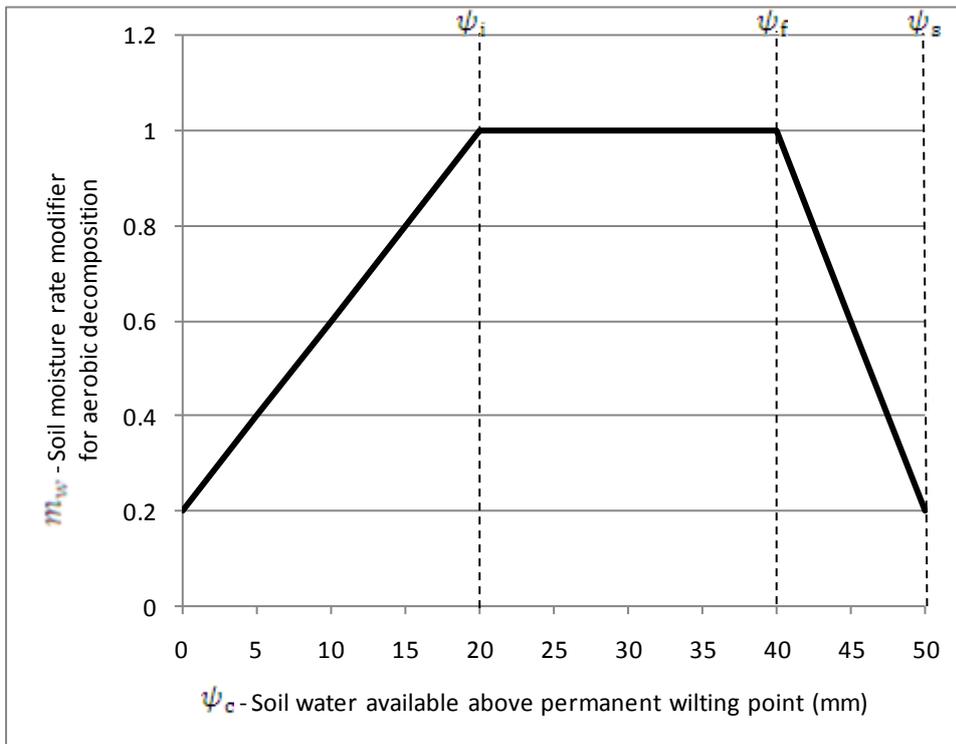


Figure 2. The soil moisture rate modifier for aerobic decomposition of soil organic matter used in ECOSSE

A3.2 Impact of soil temperature on aerobic decomposition

The rate modifier due to soil temperature, m_t , follows the equation used in RothC (Jenkinson et al. 1987),

$$m_t = \frac{47.9}{\left(1 + \exp\left(\frac{106}{T_{\text{air}} + 18.3}\right)\right)} \quad (13)$$

where T_{air} is the mean air temperature for the period in the timestep ($^{\circ}\text{C}$). A small error is introduced at depth due to using air temperature instead of soil temperature.

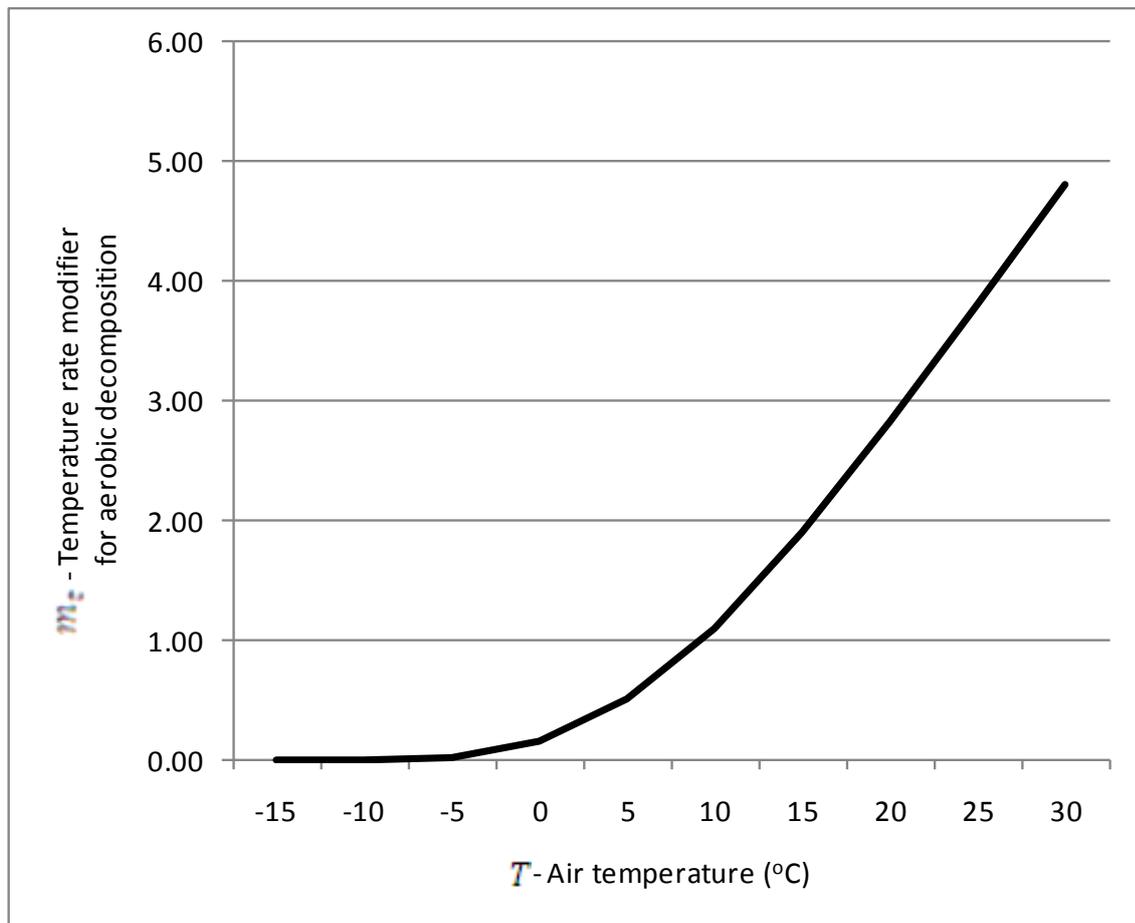


Figure 3. The temperature rate modifier for aerobic decomposition of soil organic matter used in ECOSSE

A3.3 Impact of soil pH on aerobic decomposition

A significant effect of soil pH on the rate of decomposition has been observed in many studies (e.g. Andersson and Nilsson, 2001; Hall et al. 1998; Situala et al. 1995). High soil acidity is generally considered to limit the activity of decomposers but studies that have manipulated pH in the field or laboratory have found conflicting results. This can be explained by the interaction between soil pH, organic matter decomposition and nutrient cycling (Binkley and Richter, 1987). Motavalli et al. (1995) found a positive correlation between biological activity and soil pH in soils amended with ^{14}C labelled

plant residues. Similarly, Sitaula et al. (1995) used acid irrigation to examine the effect of low pH and reported that pH 3 produced CO₂ fluxes 20 % lower than at pH 4 and 5.5, between which there was no significant difference. Persson and Wiren (1989) reported that increasing the acidity of forest soil from pH 3.8 to 3.4 reduced CO₂ evolution by 83 % and from pH 4.8 to 4 by 78 %.

These effects differ with redox conditions. Increases in pH have been reported to increase CO₂ production 1.4-fold under anaerobic conditions but decrease it by 53 % under aerobic conditions (Bridgham and Richardson, 1992). Bergman et al. (1999) compared CO₂ production rates at pH 4.3 and 6.2, and found that under anaerobic conditions rates were 21 (at 7 °C) and 29 (at 17 °C) times greater at the more neutral pH, while under aerobic conditions rates were 3 times greater at 7 °C but pH had no significant effect at 17 °C.

In a simple regression model, Reth et al. (2005) included the effect of soil pH in terms of the deviation of the soil pH (pH) from the optimum pH for decomposition (pH_{opt}), and the sensitivity of the decomposition processes in this soil to pH (pH_{sens}):

$$m_{pH} = \exp \left[- \left(\frac{pH - pH_{opt}}{pH_{sens}} \right)^2 \right] \quad (14)$$

where m_{pH} is the aerobic decomposition rate modifier according to pH. Figure 4 illustrates shows how Reth's model can be used to simulate the aerobic observations described above. The plots show that Reth's approach can accurately describe the response of aerobic decomposition to soil pH if the optimum pH for decomposition and the sensitivity to pH are known and the response is assumed to flatten off above the optimum pH and below a minimum pH. The difficulty in implementing this in a functional model is in knowing what these values should be.

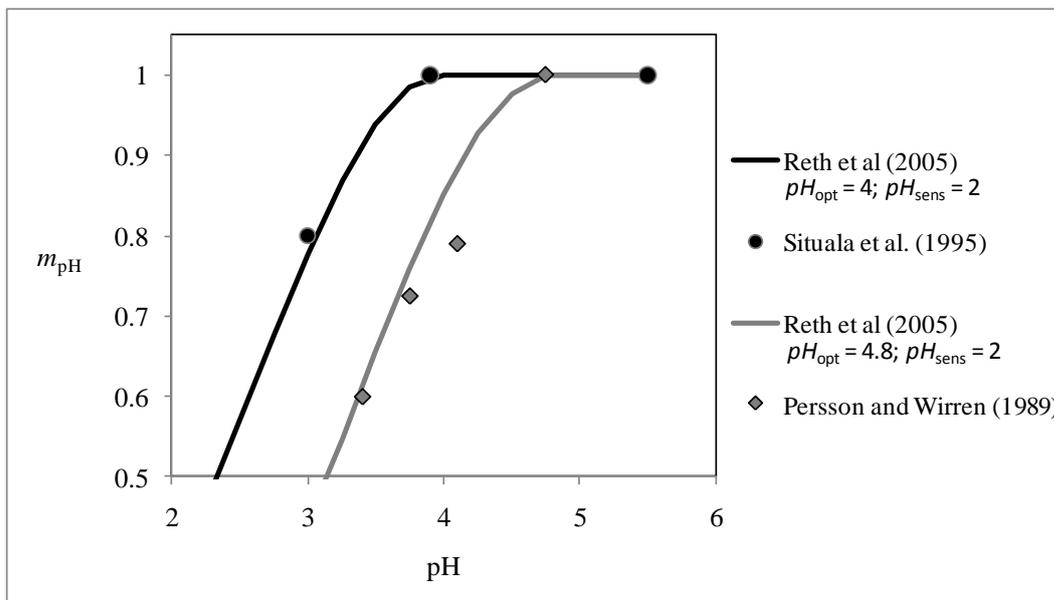


Figure 4. Fitted equation by Reth et al (2005) to the observations of changes in aerobic decomposition with pH made by Sitaula et al (1995) and Persson & Wiren (1989).

The influence of soil pH on decomposition is not implemented in the SUNDIAL or RothC models as they were originally designed to work in well-managed arable soils, and so it could be assumed that the pH was close to neutral (Bradbury et al, 1993; Coleman and Jenkinson, 1996). This assumption breaks down in natural and managed highly organic soils, where the pH is more variable. The above discussion suggests that the implementation of decomposition in ECOSSE should include a different description of the effects of pH on aerobic and anaerobic decomposition. In an approach that follows that of Reth et al. (2005), but with a simplified formula that uses more explicit terms, aerobic decomposition is described as proceeding at an optimum rate (rate modifier $m_{pH} = 1$) until the pH falls below a critical threshold (pH_{max}), after which the rate of decomposition falls to a minimum rate (rate modifier $m_{pH} = m_{pH,min}$) at pH_{min}

$$m_{pH} = m_{pH,min} + (1 - m_{pH,min}) \left(\frac{pH - pH_{min}}{pH_{max} - pH_{min}} \right) \quad (15)$$

This relationship is shown in Fig. 5. The values of $m_{pH,min}$, pH_{min} and pH_{max} can be set for each site, but by default are set at $m_{pH,min} = 0.2$, $pH_{min} = 1$ and $pH_{max} = 4.5$ as these are the values that most consistently simulate the observations described above.

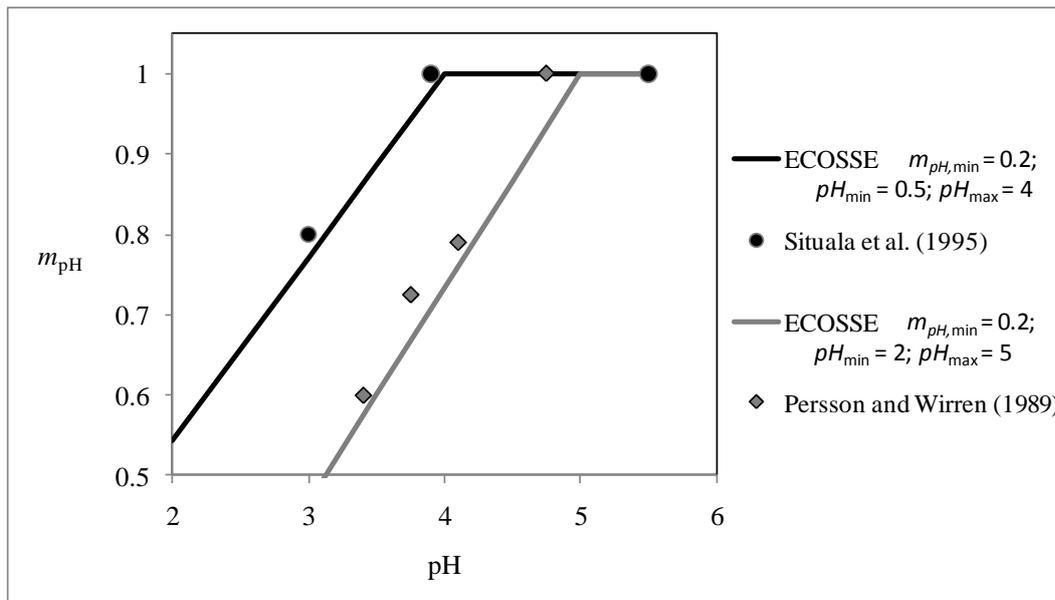


Figure 5. Anaerobic decomposition rate modifier for pH, m_{pH} , where $m_{pH,min}$ = minimum value for rate modifier according to pH; pH_{min} = pH at which rate of aerobic decomposition is at minimum rate; and pH_{max} = Critical threshold pH below which rate of aerobic decomposition starts to decrease

A3.4 Impact of crop cover on aerobic decomposition

Following work by Jenkinson (1977) on the impact of plant cover on the decomposition of ^{14}C labelled ryegrass, the rate of decomposition is slowed using a crop cover rate modifier (m_c) of 0.6 if plants are actively growing, and 1 if the soil is bare.

A3.5 Impact of nitrogen on aerobic decomposition

Following the approach used in the SUNDIAL model (Bradbury et al, 1993), N impacts the rate of aerobic decomposition through the stable C:N ratio of the BIO and HUM pools. When organic matter is added to the soil, the decomposition process is assumed to immobilise or mineralise N in order to maintain the stable C:N ratio. If the C:N ratio of the added plant material is lower than the stable C:N ratio, then sufficient N is released during the decomposition process to maintain the BIO and HUM pools at the stable C:N ratio. If the C:N ratio of the added plant material is higher than the stable C:N ratio then N is immobilised, first from the NH_4^+ pool, and then when that falls to a critical minimum level defined for the soil, from the NO_3^- pool. If N in the NO_3^- pool falls to the critical minimum level, decomposition is limited to the amount of decomposition that can be achieved while maintaining the BIO and HUM pools at the stable C:N ratio given the available mineral N.

ECOSSE differs from SUNDIAL in that it includes a variable efficiency of decomposition under N limited conditions. The micro-organisms responsible for aerobic decomposition use SOM as a source of energy, and to provide the C that is used to build biological structures. It is the amount of energy required to drive these biological processes that determines the proportion of the decomposed organic material that is retained in the soil, the efficiency of decomposition.

In N limited forest soils, it has been observed that decomposition can continue, even under N limited conditions. When N is supplied to the system, for example as fertiliser, the C content of the soil appears to increase relative to the C content of the N limited soil. It is hypothesized that this is in part due to the microorganisms “mining” the SOM for N when N is limiting, emitting the excess C as CO_2 and using the remaining N to build cell structures. When N becomes available, the micro-organisms are no longer starved of N, so can use the energetically more accessible source of N, ammonium or nitrate, rather than breaking down the SOM. This is simulated in ECOSSE by including a change to the efficiency of decomposition (E), described by the proportions of decomposing material retained as biomass and humus. The efficiency of decomposition is allowed to be reduced by as much as is required to ensure that there is sufficient available soil N to balance the C released into the BIO and HUM pools. The efficiency of decomposition clearly has a lower limit of 0; indicating all of the decomposed C will be released as CO_2 . The remaining N from the decomposing organic material is released into the soil as ammonium. If the N required for decomposition is still higher than is available from the SOM, then the rate of decomposition will be limited.

Change in pH has also been observed to result in a change in the C:N ratio of the organic matter in the soil. The stable C:N ratio is an important driver of mineralization or immobilisation of N during the decomposition of organic matter. In SUNDIAL, the stable C:N ratio of SOM is assumed to be a constant value of 8 under all conditions (Bradbury et al. 1987). The choice of a stable C:N ratio of 8 is a result of the weighted average of the C:N ratios of the decomposing fungi and bacteria in the soil. However, as the soil pH falls, the ratio of fungi to bacteria increases because fungi are more tolerant of acidic conditions. Because the C:N ratio of fungi is higher than the C:N ratio of bacteria, this change in the population is accompanied by an increase in the stable C:N ratio of the SOM. This is due to the decomposer community in the soil becoming dominated by fungi with a higher C:N ratio than bacteria. This suggests that the stable C:N ratio of the organic matter pools in ECOSSE should change with changing pH. In the absence of more detailed experimental data, a simple linear approach is used.

The proportion of bacteria in the soil, p_{bac} , is calculated as

$$p_{bac} = p_{bac,min} + (p_{bac,max} - p_{bac,min}) \left(\frac{pH - pH_{bac,min}}{pH_{bac,max} - pH_{bac,min}} \right) \quad (16)$$

where $p_{bac,min}$ is the minimum proportion of bacteria found in the soil, $p_{bac,max}$ is the maximum proportion of bacteria found in the soil, pH is the soil pH, $pH_{bac,min}$ is the pH at which minimum soil bacteria occurs, and $pH_{bac,max}$ is the pH at which maximum soil bacteria occurs.

Similarly, the proportion of fungi in the soil, p_{fun} , is calculated as

$$p_{fun} = 1 - \left(p_{bac,min} + (p_{bac,max} - p_{bac,min}) \left(\frac{pH - pH_{bac,min}}{pH_{bac,max} - pH_{bac,min}} \right) \right) \quad (17)$$

The stable C:N ratio of the SOM, $(C:N)_{stable}$, can then be calculated from the proportion of bacteria and fungi in the soil, and the typical C:N ratios of bacteria and fungi, $(C:N)_{bac} = 5.5$ and $(C:N)_{fun} = 11.5$ respectively, i.e.

$$(C:N)_{stable} = (p_{bac} \times (C:N)_{bac}) + (p_{fun} \times (C:N)_{fun}) \quad (18)$$

The change with pH in the proportion of fungi and bacteria and the stable C:N ratio of SOM is shown in Figure 6.

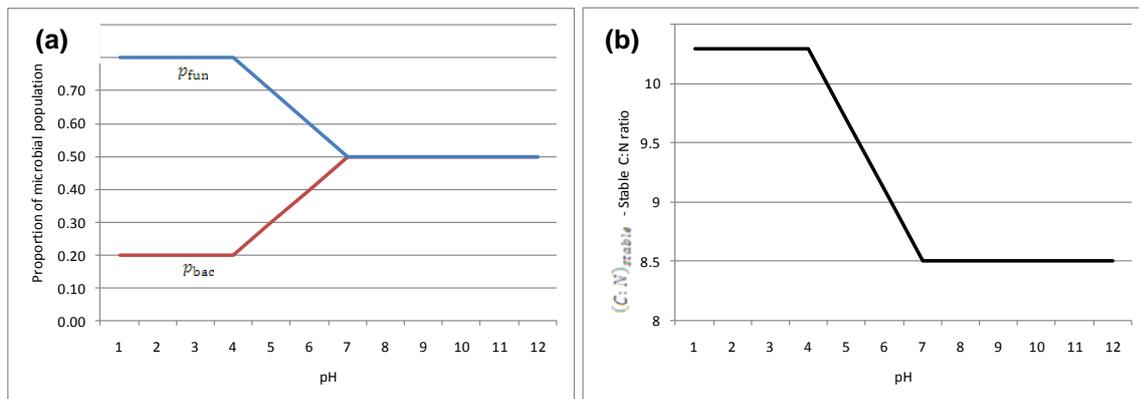


Figure 6. Calculation of change in stable C:N ratio with pH; (a) proportion of fungi and bacteria; (b) stable C:N ratio.

A3.6 Impact of clay content on aerobic decomposition

In ECOSSE, there is no rate modifying factor for clay content. Instead, following the approach used in RothC (Jenkinson, 1977) and SUNDIAL (Bradbury et al, 1993), the clay content of the soil impacts aerobic decomposition by altering the partitioning between CO_2 evolved and (BIO+HUM) formed during decomposition. In other words, the clay content is used to determine the efficiency of decomposition (E) under non-N-limiting conditions as already described in equation 4.

A3.7 Evaluation of ECOSSE simulations of aerobic decomposition

An evaluation of the ECOSSE simulations of aerobic decomposition has been completed for a range of soil conditions, in a number of different soil environments and under different land uses. This work is currently being prepared for publication and so cannot be included here. When published, a summary of the evaluation and a reference to the published paper will be provided.

A4 Anaerobic decomposition of soil organic matter pools

The process of anaerobic decomposition is included in the ECOSSE model, and is assumed to result in emissions of CH_4 . Methane is an important contributor to global warming, which is produced by methanogenic bacteria in soil when decomposition occurs under anaerobic, reducing conditions. Wetlands represent the most important natural source of methane emissions to the environment. The rate of methane emissions are often reported to increase with temperature, so there is potential for positive feedback due to climate change. This emphasises the need to understand the processes that control CH_4 emissions from wetlands and how they react to both environmental and land use changes.

The DNDC model (Zhang et al 2002) calculates CH_4 production as a function of DOC concentration and temperature, under anaerobic conditions where the soil redox potential (Eh) is predicted to be 150 mV or less. Methane oxidation is calculated as a function of soil CH_4 and Eh. Methane moves from anaerobic production zones to aerobic oxidation zones via diffusion, which is modelled using concentration gradients between soil layers, temperature and soil porosity. Methane flux via plant transport is a function of CH_4 concentration and plant aerenchyma. The density of plant aerenchyma is a function of the plant growth index, which is calculated using plant age and season days. If the density of plant aerenchyma is not well developed, or soil is non-vegetated, the efflux is determined by ebullition (bubbling). In DNDC, this is assumed to occur only at the surface level, and is regulated by CH_4 concentration, temperature, porosity, and any existing plant aerenchyma.

By contrast, to the very complex approach used in DNDC, Christensen et al (1996) described methane emissions very simply as a proportion of the total heterotrophic respiration. In ECOSSE we simulate CH_4 emissions using a simple but process-based approach. Methane emissions are calculated as the difference between CH_4 production and oxidation, the oxidation process adding to emissions of CO_2 (Figure 8).

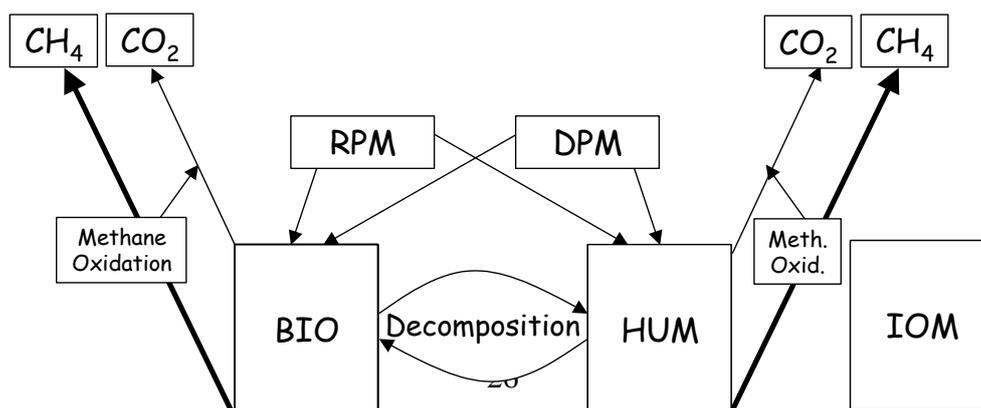


Figure 8 Structure of methane model in ECOSSE

Methane production during anaerobic decomposition is simulated using a similar pool approach as is used for aerobic decomposition. Under anaerobic conditions, the concentration of C in decomposing SOM pool at end of time step t , $[C_R]_t$, is given by

$$[C_R]_t = [C_R]_0 \left(1 - \exp(-k'_R t \times m'_w \times m'_t \times m'_c \times m'_{pH}) \right) \quad (18)$$

where k'_R is the rate constant for anaerobic decomposition of pool R (time step⁻¹); the rate constants used are assumed to be equivalent to the rate constants for aerobic decomposition as given in RothC; for DPM $k'_{DPM} = 10 \text{ yr}^{-1}$, for RPM $k'_{RPM} = 0.3 \text{ yr}^{-1}$, for BIO $k'_{BIO} = 0.66 \text{ yr}^{-1}$, and for HUM $k'_{HUM} = 0.02 \text{ yr}^{-1}$. The difference between the rates of aerobic and anaerobic decomposition is simulated through the different functions used to calculate the rate modifiers; m'_w , m'_t , m'_c and m'_{pH} are the rate modifiers that account for the impact of changes in soil moisture, temperature, crop cover and pH respectively. The form of these rate modifiers is described in the following sections. Clearly under conditions of intermediate anaerobicity, the concentration of C in the decomposition SOM pool, $[C_R]_t$, is contributed to by both the aerobic and anaerobic processes.

The production of methane, C_{CH4} (kg C ha⁻¹ timestep⁻¹ layer⁻¹) is then given by

$$C_{CH4} = (1 - p_{BIO} - p_{HUM}) \times [C_R]_0 \left(\exp(-k'_R t \times m'_w \times m'_t \times m'_c \times m'_{pH}) \right) \quad (20)$$

where p_{BIO} is the proportion of decomposing materials partitioned to biomass, and p_{HUM} is the proportion partitioned to humus. The values of p_{BIO} and p_{HUM} are calculated from the efficiency of decomposition, E , as shown in equations 6 and 7.

The oxidation of methane ($C_{CH4 \rightarrow CO2}$) is calculated from methane production as

$$C_{CH4 \rightarrow CO2} = (1 - \tau) \times \gamma d \times C_{CH4} \quad (21)$$

where τ is a transport factor (for non-transporters $\tau = 0$; for transporting non-sedges $\tau = 0.25$; for transporting sedges $\tau = 1$ (Kettunen, 2002)); γ is a soil dependent factor that accounts for different rates of diffusion and oxidation (derivation is described in the following sections); and d is the depth (cm).

A4.1 Impact of soil water on anaerobic decomposition

Methane emissions only occur in strongly anoxic soils (Le Mer and Roger 2001). Therefore the rate modifier is assumed to be non-zero only at water contents over field capacity.

Following the approach used wetlands DNDC (Zhang et al, 2002), the rate of methane production is assumed to increase exponentially above field capacity (see Figure 9) and is calculated as

$$m'_w = c_2 \times \exp\left(\left(c_1 \times (\psi_c - \psi_i)\right) - 1\right) \quad (22)$$

where ψ_c is the soil water deficit (mm layer⁻¹); ψ_i is the amount of water held in a layer between field capacity and the soil at -100 kPa (mm layer⁻¹) and c_1 and c_2 are fitted constants ($c_1 = 0.5$ and

$c_2 = \frac{1}{\exp((0.5 \times (\psi_s - \psi_i)) - 1)}$ (where ψ_s is the amount of water held in a layer between saturation and the permanent wilting point (mm layer⁻¹)). The rate modifier is shown in figure 8.

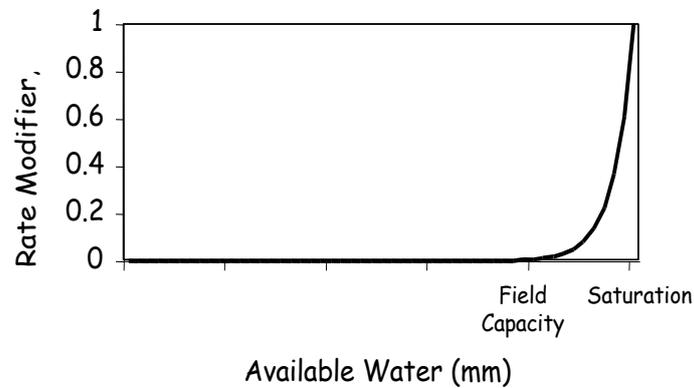


Figure 9 Response of anaerobic decomposition to available water in the soil

A4.2 Impact of soil temperature on anaerobic decomposition

Field measurements of changes in methane emissions with temperature can be difficult to unravel, as many confounding factors can contribute to the observed emissions. Christensen et al (2002) report that mean seasonal temperature is the best predictor of methane fluxes on a large scale. Hargreaves et al (2001) observed an exponential relationship between surface temperature (0-10 cm) and methane flux for measurements without a thaw period, with a Q_{10} of 4, while Rask et al (2002) found a linear relationship between the same factors in a shallow bay area of a fen. Hargreaves & Fowler (1998) reported a linear relationship with temperature between 7 and 11°C, with a slope of $5 \mu\text{mol CH}_4 \text{ m}^{-2} \text{ h}^{-1} \text{ }^\circ\text{C}^{-1}$ for peat wetlands in Caithness, Scotland. Other workers have also reported significant relationships between soil temperature in the surface layer and methane flux, in wet tundra sites (Christensen et al, 1995) and subalpine wetlands (Wickland et al, 1999, 2001). Although these field observations describe different responses, a positive relationship between methane emissions and temperature is generally observed (Figure 10).

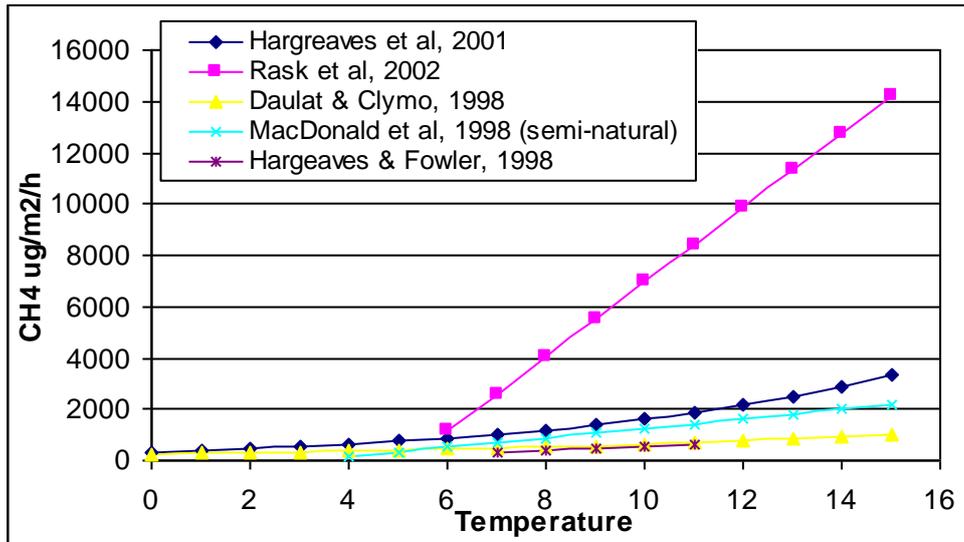


Figure 10 Reported responses of methane emissions to temperature

Micro- and mesocosm measurements provide a less complex picture, allowing confounding factors to be removed from the experimental setup. Daulat & Clymo (1998) reported an exponential relationship between soil temperature at 5 cm depth and mean methane flux in peat cores from Scotland. Lloyd et al (1998) commented on the high sensitivity of methane fluxes from Scottish peat cores to temperature, reporting a Q_{10} of 3 in the dark. MacDonald et al (1998) also report Q_{10} values of around 3 (between 5 and 15°C) for relationships between peat temperature and methane flux from peat cores from Northern Scotland, which are linear under semi-natural conditions, and exponential under controlled conditions of constant humidity and light.

Following the model of Kettunen (2002), the temperature rate modifier is given by the equation:

$$m'_t = \frac{47.91}{\exp\left(\frac{125}{(T_{\text{soil}} + 18.27)}\right) + 1} \quad (23)$$

where T_{soil} is the temperature of the soil layer (°C)

In agreement with the observations of Daulat & Clymo (1998), Lloyd et al. (1998) and MacDonald et al. (1998), this relationship shows a Q_{10} value close to 3 between 5 and 15°C (see Fig. 11).

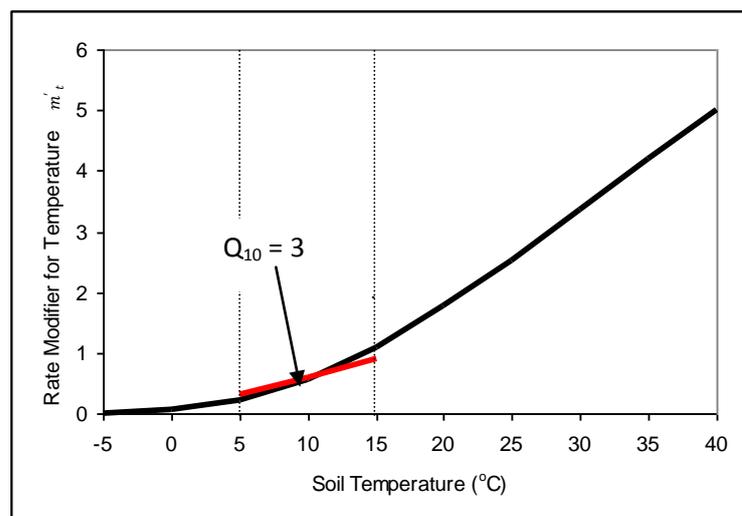


Figure 11 Response of anaerobic decomposition to soil temperature

A4.3 Impact of soil pH on anaerobic decomposition

Methanogenic bacteria are generally reported to exhibit maximum activity under neutral or slightly higher pH conditions (Garcia et al, 2000) and to be very sensitive to variations in soil pH (Wang et al, 1993). Garcia et al (2000) reported that 68 species of methanogenic bacteria could not grow at a pH lower than 5.6. However, methane producers can adapt to more acidic environments, as many studies have recorded methanogenic activity in soils with a lower pH. Williams and Crawford (1985) reported that a mixed bacterial culture from a Minnesota peatland produced methane at pH values between 3 and 4. Dunfield et al (1993) investigated methane production in peat soil samples from temperate and subarctic areas (pH 3.5–6.3) and reported an optimum production rates at pH of 5.5 to 7.0. Inubushi et al (2005) reported a positive correlation between methane production activity and soil pH ($r^2 = 0.802$, $P < 0.01$) for peat soil samples from a temperate Japanese wetland, which had a pH range of 5-7. However, more acidic Indonesian peat soils, which ranged from pH 3.9-5, showed no correlation with pH (Inubushi et al, 2005). Depth can also affect the influence of soil pH on methane production. Williams and Crawford (1984) found that a pH increase from 3.2 to 5.8 increased the methane production of an incubated peat from a Minnesota peatland by 1.5 fold, for samples from 10 cm depth, and 2.2 fold for samples from 60 cm depth. To complicate things further, some studies have reported negative relationships. Bergman et al (1999) reported a negative effect of pH on methane production in incubations of peat soil from a Swedish mire, but it was only statistically significant for one of two years data. Bergman et al (1999) reported both positive and negative relationships with pH for peat originating from different plant communities within the same mixed mire site in Sweden, and suggested that conflicting results may be due to competition for hydrogen between methanogens and homoacetogens, increasing pH favouring the later since it increases the degree of dissociation of acetate, or due to differences in cation exchange capacity (CEC).

It is clear that the response of methane production to pH is very complex. Some of these conflicting results may have been confounded by methane oxidation. However, from the above results it can be stated that the rate of methane production is usually at an optimum ($m'_{pH} = 1$) at around pH 7 (Garcia et al, 2000; Wang et al, 1993), and is close to the optimum between pH 5.5 –7 (Dunfield et al., 1993), decreasing to close to zero at around pH 3 (Williams & Crawford, 1984, 1985; Dunfield et al., 1993). This response can be simulated using a sigmoid relationship),

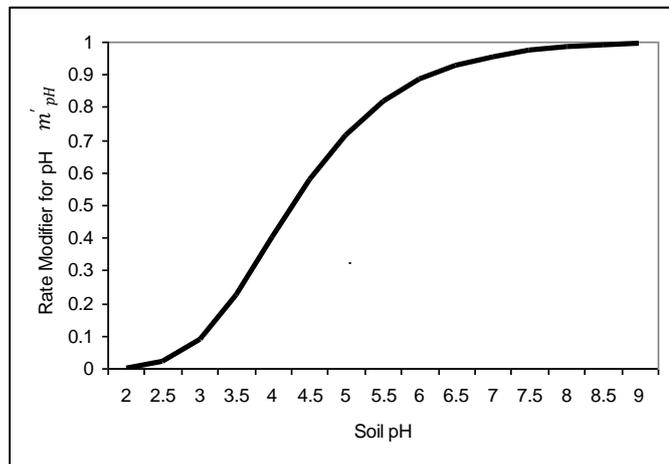


Figure 12. Response of anaerobic decomposition to soil pH

$$m'_{pH} = \left(1.0^{1/c_4} + \exp(c_3 \times pH) \right)^{c_4} \quad (24)$$

where pH is the measured pH of the soil layer, and c_3 and c_4 are constants ($c_3 = -1$, and $c_4 = -50$). The relationship between m'_{pH} and pH is shown in Fig. 12.

A4.4 Impact of crop cover on anaerobic decomposition

Anaerobic decomposition is assumed to follow the same response to crop cover as used for aerobic decomposition.

A4.5 Impact of nitrogen on anaerobic decomposition

Nitrogen is assumed to have the same impact on anaerobic decomposition as it does on aerobic decomposition.

A4.6 Impact of clay content on anaerobic decomposition

As for aerobic decomposition, the clay content of the soil impacts aerobic decomposition by altering the partitioning between CO₂ evolved and (BIO+HUM) formed during decomposition.

A4.7 Impact of oxygen on methane emissions

Water table depth is one of the main factors controlling methane emissions as it determines the position of the boundary between the anaerobic and aerobic zones. When the water table is below the soil surface, oxidation of methane becomes a major controlling variable for methane efflux (Christensen et al, 2000). As a result, a lower water table decreases methane emission (Blodau et al, 2004) and draining peats may even convert the soil to a net methane sink (Blodau & Moore, 2003; Huttunen et al, 2003; Maljanen et al, 2002). Hargreaves & Fowler (1998) measured methane fluxes over a peat wetland in Caithness and related them to water table depths in different areas of the bog. They found a negative linear relationship between

linear relationship between depths of around 8-17 cm. Daulat & Clymo (1998) also report a linear relationship between water table depth and methane emission, with depths of more than 15-20 cm below the soil surface stopping peat cores from being a net emitter of methane (Fig. 13).

MacDonald et al (1998) found a reduction in methane emissions from Scottish peat

cores with increasing water table depth, but in this case, the observed relationship is a decay curve and the cores do not become net sinks for methane even when the water table is 40 cm below the surface. Moore & Dalva (1993) found a negative logarithmic correlation with water table depth, down to 60 cm, in cores of peatland. Where the water table is above the surface, oxidation can also reduce methane emissions, particularly if light availability allows benthic photosynthetic activity (Le Mer & Roger, 2001).

If it can be assumed that methane oxidation is close to zero when the water table is at the surface, the soil factor accounting for diffusion and oxidation of methane (ν) can be calculated from the

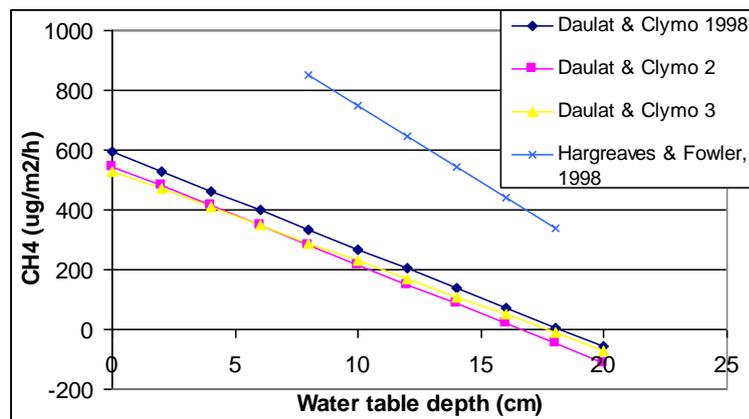


Figure 13. Reported responses of methane emissions to water table depth

depth (in cm) at which methane emissions cease and the soil becomes a net methane sink (d_{sink}) as follows:

$$v = \frac{1}{d_{\text{sink}}} \quad (25)$$

This results in a value of $v = 0.056 \text{ cm}^{-1}$ for the soils of Daulat and Clymo (1998), and $v = 0.04 \text{ cm}^{-1}$ for the soils of Hargreaves and Fowler (1998). The methane emissions calculated in this way are shown in Fig. 14. Further work is required to determine the relationship between soil type and the depth at which the soil becomes a net methane sink.

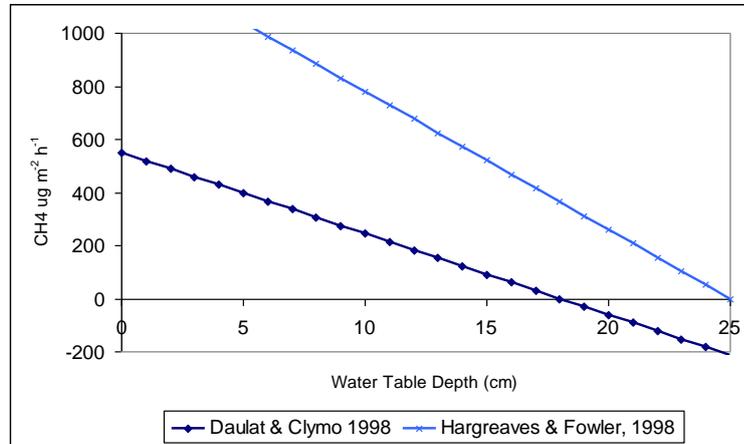


Figure 14. Reduction in methane emissions with depth of water table, as calculated by ECOSSE

Methane oxidizing bacteria

(methanotrophs) are more tolerant to pH variations than methanogens, with a reported optimum pH of 5.0 to 6.5 in temperate and subarctic peats (Dunfield et al, 1993), and have been discovered in peat soils below pH 4.7 using molecular ecological methods (MacDonald et al, 1996). However, Hutsch et al (1994) reported that, in a non-fertilised permanent grassland at the Rothamsted experimental station, a decrease in pH from 6.3 to 5.6 reduced methanotrophy by almost half. As a first approximation, it is assumed that methane oxidation is not influenced by soil pH.

A4.8 Evaluation of ECOSSE simulations of anaerobic decomposition

An evaluation of the ECOSSE simulations of anaerobic decomposition has been completed for a range of soil conditions, in a number of different soil environments and under different land uses. This work is currently being prepared for publication and so cannot be included here. When published, a summary of the evaluation and a reference to the published paper will be provided.

A5 Nitrogen transformations

A5.1 Mineralisation / Immobilisation

As already described in section A3.5, mineralisation / immobilisation turnover is calculated following the approach used in the SUNDIAL model by Bradbury et al (1993), modified to allow for N limited conditions.

A5.2 Nitrification

DNDC predicts nitrification rates by tracking nitrifier activity and NH_4^+ concentration. Growth and death rates of nitrifying bacteria are calculated as a function of DOC concentration, temperature and

moisture, based on Blagodatsky & Richter (1998) and Blagodatsky et al (1998). Nitrification rates are then predicted as a function of the nitrifier biomass, NH_4^+ concentration and pH. Nitrification-induced NO and N_2O production are calculated as a function of nitrification rate and temperature (Li, 2000).

NGAS takes a much simpler approach, calculating nitrification directly as a function of water filled pore space (WFPS), pH, temperature and soil NH_4^+ levels. Each of the four variables controls the fraction of nitrification that occurs under the given conditions. The effect of WFPS is based on Doran *et al* (1988) and is a function of soil texture. It consists of two bell-shaped curves where maximum nitrification occurs at of 0.55 for the sandy soils and 0.61 for medium and fine-textured soils. The effect of temperature is an exponential function with a Q_{10} of 2, based on the work of Sabey et al (1959):

$$m''_t = -0.06 + 0.13 \exp(0.07 \times T_{\text{air}}) \quad (26)$$

where m''_t describes the effect of temperature on nitrification, and T_{air} is the air temperature at the soil surface ($^{\circ}\text{C}$).

The effect of pH on nitrification is an S-shaped curve based on data presented by Gilmore (1984) and Motavalli et al (1995), where the optimum pH is taken to be pH 7.

Finally, NH_4^+ affects nitrification based on Malhi and McGill (1982):

$$m''_{\text{NH}_4} = 1 - \exp(-0.0105 \times N_{\text{NH}_4}) \quad (27)$$

where m''_{NH_4} is the effect of NH_4^+ on the nitrification fraction and N_{NH_4} is the concentration of ammonium in the soil.

Maximum nitrification is set as a constant based on field data from Mosier et al (1991), although (Parton et al 1996) suggests it varies as a function of soil texture. None of these factors are parameterised for highly organic or very acidic soils. Frolking et al (1998) modified these relationships when incorporating NGAS into CENTURY, changing the temperature curve according to Malhi and McGill (1982), specifying a maximum nitrification rate of 10 % of soil NH_4^+ per day, and setting N_2O emissions as 2 % of nitrification.

Using a similar but simpler approach, nitrification is simulated in ECOSSE according to the amount of ammonium in the soil layer, and is modified according to the temperature, moisture content and soil pH. The amount of N nitrified, N_n , is calculated (in kg N ha^{-1}) using the expression for nitrification developed by Bradbury et al (1993), i.e.

$$N_n = N_{\text{NH}_4} \times \exp(-0.6 \times m''_t \times m''_w \times m''_{\text{pH}}) \quad (28)$$

where N_{NH_4} is the amount of ammonium in the soil (kg N ha^{-1}), m''_t is a rate modifier due to soil temperature, m''_w is a rate modifier due to soil water, and m''_{pH} is a rate modifier due to soil pH.

The expression for the water rate modifier is adapted from that used by Bradbury et al. (1993) to include reduced nitrification in anaerobic soils, i.e. below field capacity, the rate modifier follows the equation derived for the SUNDIAL model (Bradbury et al. 1993), which assumes aerobic decomposition proceeds at its maximum rate as the soil dries from field capacity to the amount of water held at -100 kPa, but then decomposition is inhibited below -100 kPa until the soil is at its permanent wilting point:

$$m''_w = 1 - \frac{((1 - m''_{w0}) \times (\psi_f - \psi_c - \psi_i))}{\psi_f - \psi_i} ; \text{ (if } (\psi_f - \psi_c) > \psi_i, m''_w = 1) \quad (19)$$

where m''_{w0} is the rate modifier at permanent wilting point = 0.2, ψ_c is the amount of water held in a particular soil layer above the permanent wilting point (mm layer^{-1}), ψ_i is the amount of water held between field capacity and -100 kPa (mm layer^{-1}), and ψ_f is the amount of water held between field capacity and the permanent wilting point (mm layer^{-1}). Above field capacity, the rate modifier is assumed to follow a linear decline to the minimum rate of 20%, i.e. $m''_{w0} = 0.2$, at saturation.

$$m''_w = 1 - \frac{((1 - m''_{w0}) \times (\psi_c - \psi_f))}{\psi_s - \psi_f} \quad (20)$$

where ψ_s is the water content between saturation and permanent wilting point. A linear decline is

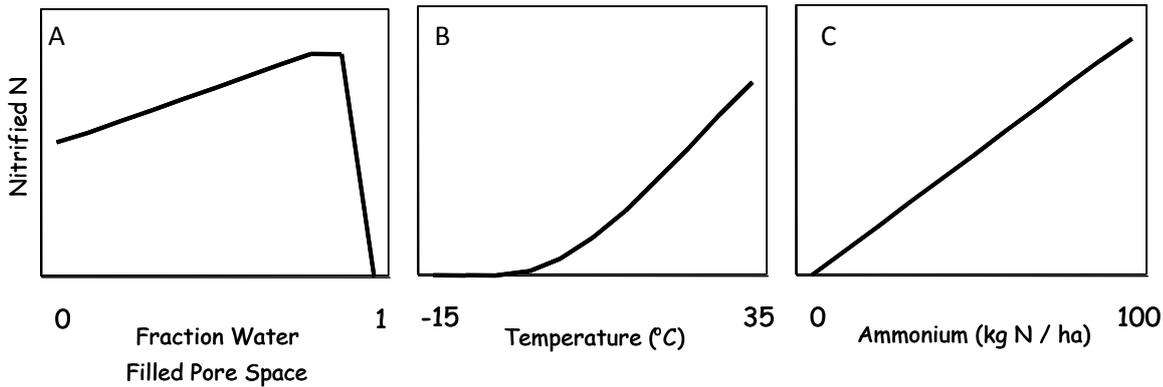


Figure 15. Response in amount of N nitrified to (A) soil water content; (B) temperature; (C) ammonium content

used because there is insufficient evidence to suggest a more refined relationship; in the absence of data suggesting a significant improvement can be achieved by using a more complex equation, the simplest form should be used to maintain model parsimony.

The response of nitrification to the soil water content is shown in Fig. 15 (A).

The expression for the temperature rate modifier, m''_t , is given by the expression used by Bradbury et al (1993) for both mineralization and nitrification, i.e.

$$m''_t = \frac{47.9}{\left(1 + \exp\left(\frac{106}{T_{\text{air}} + 18.3}\right)\right)} \quad (21)$$

where T_{air} is the air temperature ($^{\circ}\text{C}$).

The response to air temperature is shown in Fig. 15 (B), and the response to ammonium is shown in Fig. 15 (C).

The pH response function suggested by Parton et al (1996) was used. In this model, rate is about 1 (unmodified) at about neutral pH, but decreases below neutral:

$$m''_{\text{pH}} = 0.56 + \frac{\tan^{-1}(3.14 \times 0.45 \times (\text{pH} - 5))}{3.14} \quad (22)$$

Conversion of ammonium to nitrate by nitrification is accompanied by gaseous losses of N due to complete and partial nitrification. The gaseous losses as NO and N₂O are calculated using linear relationships shown in Fig. 16.

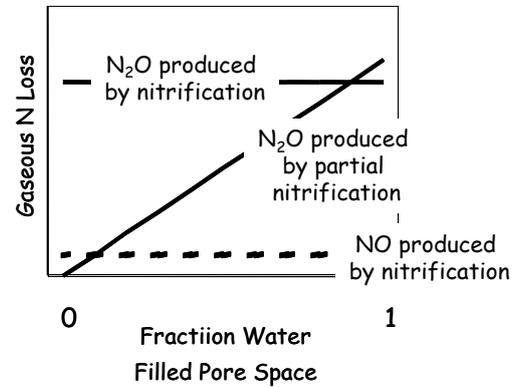


Figure 16. Partitioning of N lost by denitrification into N₂ and N₂O with respect to soil water and nitrate content

The amount of gas emitted as N₂O during nitrification, N_{n,N_2O} , is given (in kg N ha⁻¹) by

$$N_{n,N_2O} = \left(\left(n_f \times \frac{\psi_c}{\psi_f} \right) + \left(n_{\text{gas}} \times (1 - n_{\text{NO}}) \right) \right) \times N_n \quad (23)$$

where $n_f = 0.2$ is the proportion of N₂O produced due to partial nitrification at field capacity, $n_{\text{gas}} = 0.02$ is the proportion of full nitrification lost as gas, and $n_{\text{NO}} = 0.1$ is the proportion of full nitrification gaseous loss that is NO.

Similarly, the amount of gas emitted as NO during nitrification, $N_{n,NO}$ is given (in kg N ha⁻¹) by

$$N_{n,NO} = n_{\text{gas}} \times n_{\text{NO}} \times N_n \quad (24)$$

A5.3 Denitrification

Denitrification is a process that responds to changes in the system on a shorter timescale than many of the other C and N turnover processes. As a result, denitrification is difficult to measure accurately, and difficult to simulate without short-term and detailed input data. As a result, many models of

denitrification have high data requirements. The aim in ECOSSE is to develop a model that will simulate processes to the required accuracy but without the need for detailed data that will not be available at the large scale.

The denitrification sub-model of DNDC calculates N₂O and NO production, consumption and diffusion during rainfall, irrigation and flooding events. DNDC simulates relative growth rates of nitrate, nitrite, NO, and N₂O denitrifiers based on soil Eh, and concentration of DOC and N oxides. The soil matrix is divided into aerobic and anaerobic zones using an "anaerobic balloon", which swells and shrinks in response to oxygen diffusion and consumption in the soil profile. Substrates allocated to the anaerobic zone of the profile are then used to determine the denitrifier growth rates based on a simple function of multinutrient-dependent growth (based on Bader, 1978). The death rate is a constant fraction of total denitrifier biomass. Relative growth rates for denitrifiers with different substrates are assumed to be independent, and competition takes place via the common DOC substrate (based on Leffelaar & Wessel, 1988). Substrate consumption rates are calculated using growth rates and biomass. NO, N₂O and N₂ fluxes are calculated using the basic laws of kinetics, as denitrification is a typical sequential reaction. As intermediates of the reactions, NO and N₂O fluxes are determined by rates of production, consumption and escape from the reacting system. Escape is controlled by diffusion rate, a function of soil porosity, moisture, temperature and clay content (Li, 2000).

The CENTURY denitrification model in NGAS is based on data from Weier et al (1993). Total denitrification N gas fluxes (N₂ + N₂O) are a function of soil heterotrophic respiration rate (index of carbon availability), soil NO₃⁻ levels, and soil water filled pore space. Soil NO₃⁻ levels and respiration rate determine the maximum total N gas flux according to s-shaped curves fitted to experimental data. This maximum is then reduced by a fraction determined by water filled pore space, as a function of soil texture. Maximum denitrification occurs where water filled pore space is 0.9 or above. Below this value, denitrification is reduced exponentially, with fine soils declining most rapidly, followed by medium and then coarse soils. Denitrification drops to zero at water filled pore space of 0.6 for fine soils, 0.5 for medium and 0.4 for coarse. Total denitrification N gas flux is then partitioned into N₂ and N₂O as a function of soil NO₃⁻, WFPS and soil respiration (Parton et al, 1996).

In ECOSSE, a simpler approach is used in which total denitrification is simulated as a proportion of the nitrate content of the layer, modified according to water content and biological activity of the soil (as described by CO₂ release during decomposition). The denitrified N is then divided into N₂, N₂O and NO according to the water and nitrate content of the soil. The total loss of N due to denitrification is given by

$$N_d = m'''_{NO_3} \times m'''_w \times m'''_b \times N_{NO_3} \quad (25)$$

where N_d is the amount of nitrogen emitted from the soil during denitrification (kg N ha⁻¹); m'''_{NO_3} modifies this amount depending on the nitrate level, m'''_w depending on the water content, and m'''_b depending on the biological activity of the soil; and N_{NO_3} is the amount of nitrate in the soil (kg N ha⁻¹ layer⁻¹).

The nitrate modifier, m'''_{NO_3} , is based on the model developed by Henault and Germon (2000), i.e.

$$m'''_{NO_3} = \frac{N_{NO_3}}{(3.3 \times 5) + N_{NO_3}} \quad (26)$$

The response of the denitrification process to the amount of nitrate in the soil is shown in Fig. 17 (A).

The water modifier, m'''_w , is based on the fitted equation of Grundmann and Rolston (1987), i.e.

$$m'''_w = \left(\frac{(\psi_c/\psi_f) - 0.62}{0.38} \right)^{1.74} \quad (27)$$

where ψ_c is the calculated water content and ψ_f is the field capacity maximum water content of the soil (mm layer^{-1}). The response of the denitrification process to the soil water content is shown in Fig. 17 (B).

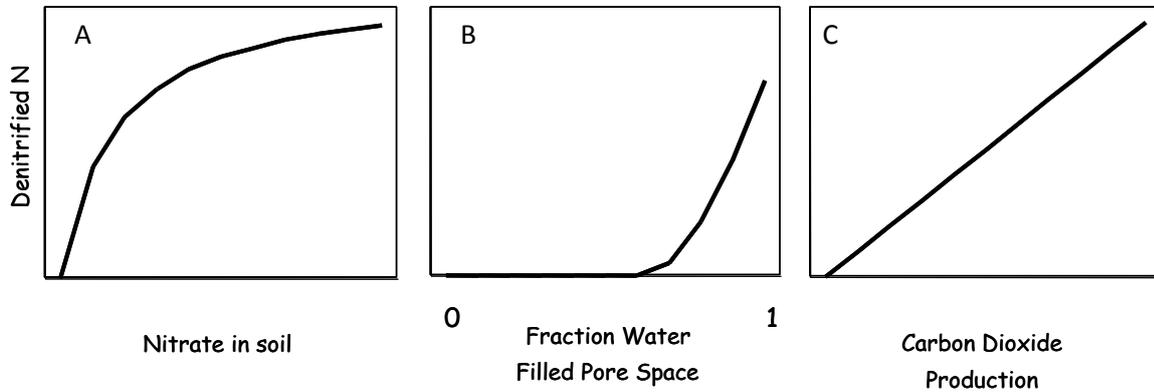


Figure 17. Response in amount of N emitted due to denitrification to (A) nitrate in soil; (B) soil water content; (C) biological activity

The biological activity modifier, m'''_b , is based on the relationship developed by Bradbury et al (1993), i.e.

$$m'''_b = 0.005 \times C_{CO_2} \quad (28)$$

where C_{CO_2} is the amount of CO_2 produced during mineralization ($\text{kg C ha}^{-1} \text{ timestep}^{-1}$). This acts as a surrogate measure of the soil biological activity. The response of the denitrification process to the soil biological activity is shown in Figure 17 (C).

The N lost by denitrification, N_d , is partitioned into N_2 and N_2O using simple linear relationships shown in Figure 18.

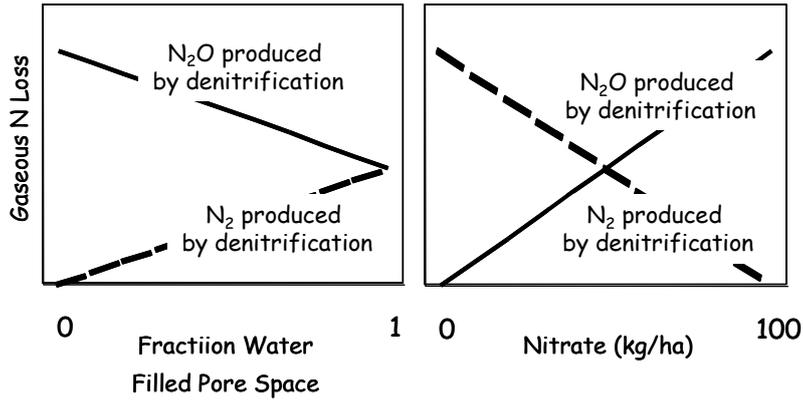


Figure 18. Partitioning of N lost by denitrification into N_2 and N_2O with respect to soil water and nitrate content

The amount of N_2 gas lost by denitrification, N_{d,N_2} , is given (in $kg\ N\ ha^{-1}$) by

$$N_{d,N_2} = p_w \times p_{NO_3} \times N_d \quad (29)$$

where N_{d,N_2} is amount of N_2 gas lost by denitrification ($kg\ N\ ha^{-1}$), p_w proportions denitrification into N_2 according to the water content of the soil, ($p_w = p_{N_2,f} \times \frac{\psi_c}{\psi_f}$ where $p_{N_2,f} = 0.5$ is the proportion of denitrified N lost as N_2 at field capacity), and p_{NO_3} proportions denitrification into N_2 according to the nitrate content of the soil, ($p_{NO_3} = 1 - \left(\frac{N_{NO_3}}{N_d \times d_0}\right)$ where $p_{N_2,0} = 0.1$ is the proportion $\frac{N_{NO_3}}{N_d}$ at which N_2 emission falls to zero and all denitrified N is lost as nitrate).

The amount of N_2O gas lost by denitrification, N_{d,N_2O} , is similarly calculated (in $kg\ N\ ha^{-1}$) by the following expression,

$$N_{d,N_2O} = \left(1 - (p_w \times p_{NO_3})\right) \times N_d \quad (40)$$

A5.4 Nitrate leaching

In SUNDIAL-MAGEC, the soil is divided into different layers for the different components of the soil: ammonium is simulated in 50cm layers down the soil profile; SOM is simulated in 25cm layers to a maximum depth of 50cm; and nitrate is simulated in 5cm layers for the top 50cm, followed by 50cm layers for the remainder of the profile. This structure does not allow C and N turnover in deep organic soils to be simulated. In ECOSSE, the layers are unified into 5cm layers throughout, so allowing C and N turnover to be simulated to depth. The soil parameters are also described in 5cm layers, so allowing more detailed descriptions of soil profile characteristics to be included. This is important in highly organic soils where the organic layer can be very deep.

A5.5 Leaching of dissolved organic matter

Dissolved Organic Carbon (DOC) is a potentially important component of carbon export from the soil system under highly organic conditions. Dissolved Organic Nitrogen (DON) is closely linked to the

production of DOC, and Jørgensen & Richter (1992) demonstrated that the two soil characteristics must be considered together in order to avoid unrealistic simulations of carbon or nitrogen concentration in the soil. Evans et al. (2005) give a convincing argument that DOC production in organic soils is increasing, not due to climate change-induced oxidation, but instead as a result of soils recovering from acid deposition, which suppresses DOC solubility. They demonstrate a link between increased temperature, declining sulphur deposition and sea-salt loading. Strong links are already known to exist between soil water pH and DOC solubility, with an inverse relationship between mineral and organic acid export from soils (Krug and Frink, 1983). Palmer et al. (2001) used a combination of stable isotope and ¹⁴C-dating to identify the main sources and processes controlling DOC production in a temperate non-forested watershed underlain by mostly organic and podzolic soils. They found that the main source of DOC was the readily-decomposable carbon, such as leaf litter, rather than the longer term storage of SOM. They also showed that wetter soils export more 'recent' carbon than dry soils: DOC from dry soils contains more of the older carbon than does DOC from wet soils.

DyDOC is a model of DOC production that utilises a layered soil description (Michalzik et al., 2003), and contains different organic fractions. Three processes are represented in DyDOC: hydrology, metabolism and sorption. Hydrology is modelled in terms of macropores and micropores, between which dissolved organic carbon diffuses. Metabolism is modelled using relatively simple relationships to define the transformations between the three pools of organic carbon, with only temperature being a variable. Sorption occurs to and from soil solids from the different pools, and is controlled by DOC type, soil solution pH and cation content, and the nature of the soil solids (texture etc.). In ECOSSE, we follow a similar approach, simulating the hydrological, metabolical and sorptive processes using the 5 soil organic matter pools: decomposable and resistant plant material, soil biomass, humus, and inert organic matter. A further organic matter pool is introduced, containing the DOC and DON that is in solution (see Fig. 19).

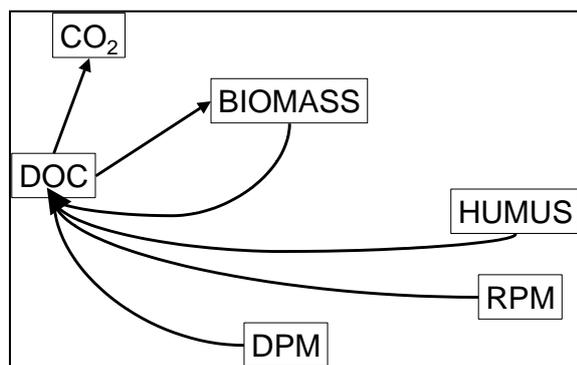


Figure 19. Pool structure for DOC production and uptake

This dissolved component is then susceptible to leaching by the same processes as already exist in the model to describe leaching losses. According to the model of Aguilar & Thibodeaux (2005a; 2005b), there are two fractions of DOC, one fraction that is readily available in the soil solution at all times, and another that is created from slower decomposition processes. This observation is consistent with the transfer into the DOC pool during decomposition of material from the rapidly turning over biomass and plant material pools, as well as from the more slowly turning over humus

pool. In DyDOC production by metabolism is calculated using a Q_{10} relationship with a rate dependent only on temperature:

$$\Delta C_R = -k''''_R \times Q_{10}^{T_{air}/10} \times C_R \times \Delta t \quad (41)$$

where k'''_R is the rate constant for DOC production specific to the pool; Q_{10} is a constant, usually set to 2.0; T_{air} is the average air temperature ($^{\circ}C$); C_R is the amount of carbon in the pool ($kg\ C\ ha^{-1}$) and t is the size of the timestep.

In ECOSSE we differentiate the equation, and include rate modifiers for moisture (m''''_w), temperature (m''''_t), crop cover (m''''_c) and pH (m''''_{pH}) as used in the existing calculation of SOM decomposition. The amount of DOC produced ($C_{pool \rightarrow DOC}$) by a given pool is then calculated as:

$$C_{R \rightarrow DOC} = C_R \times \exp(k'''_R \times m''''_w \times m''''_t \times m''''_c \times m''''_{pH}) \quad (42)$$

where k'''_R is set to $0.0001\ day^{-1}$ for decomposable plant material; $0.000005\ day^{-1}$ for resistant plant material; $0.00005\ day^{-1}$ for soil biomass; and $0.000002\ day^{-1}$ for humus.

The moisture modifier (m''''_w) is calculated from the available water at saturation (ψ_s), the available water at field capacity (ψ_f) and the actual available water in the 5cm layer (ψ_c) (all in mm) as follows:

$$\text{if } (\psi_f - \psi_c) > 4\text{mm then } m''''_w = (1 - m''''_{w0}) \times \frac{(\psi_f - \psi_c - 4)}{\psi_f - 4} \quad (43)$$

$$\text{if } (\psi_f - \psi_c) \leq 4\text{mm then } m''''_w = 1 \quad (44)$$

$$\text{if } (\psi_f - \psi_c) < 0\text{mm then } m''''_w = \frac{(\psi_s - \psi_c)}{\psi_s - \psi_f} \quad (45)$$

The temperature rate modifier is calculated from the temperature of the soil layer in $^{\circ}C$ (T_{soil}) as follows:

$$\text{if } T_{soil} < -10\ ^{\circ}C \text{ then } m''''_t = 0 \quad (46)$$

$$\text{if } T_{soil} \geq -10\ ^{\circ}C \text{ then } m''''_t = \frac{47.91}{\left(1 + \exp\left(\frac{106.06}{(T_{soil} + 18.27)}\right)\right)} \quad (47)$$

The crop rate modifier is set as follows:

$$\text{if no crop, } m''''_c = 1.0 \quad (48)$$

$$\text{if no crop, } m''''_c = 0.6 \quad (49)$$

Finally, the pH rate modifier is calculated as discussed in section A4.3 as

$$m''''_{pH} = \frac{pH - pH''''_{min}}{pH''''_{max} - pH''''_{min}} \quad (50)$$

where pH is the pH of the soil layer; and pH''''_{min} and pH''''_{max} are the pH values at which the minimum and maximum rate of decomposition occur respectively.

The carbon in the DOC pool (C_{DOC}) can further decompose to produce additional biomass ($C_{\text{DOC} \rightarrow \text{BIO}}$) following a similar expression to the above:

$$C_{\text{DOC} \rightarrow \text{BIO}} = C_{\text{DOC}} \times \exp(k_{\text{DOC}} \times m''''_w \times m''''_t \times m''''_c \times m''''_{pH}) \quad (51)$$

where k_{DOC} is set to 0.005 day^{-1} .

The decomposition to biomass produces a fixed proportion of carbon dioxide ($C_{\text{DOC} \rightarrow \text{CO}_2}$), i.e.

$$C_{\text{DOC} \rightarrow \text{CO}_2} = f_{\text{eff}} \times C_{\text{DOC} \rightarrow \text{BIO}} \quad (52)$$

where f_{eff} is a fraction representing the efficiency of decomposition, and is set according to soil type to the same value as used in the decomposition routines. Having calculated the changes in carbon, the transformations in DON are calculated using the C:N ratio of the decomposing pool. Leaching of DOC takes place only for the portion that is not sorbed onto soil solids. The proportional availability ($C_{\text{DOC,sol}}$) of DOC is dependent on pH using the following relationship

$$C_{\text{DOC,sol}} = C_{\text{DOC}} \times \frac{(pH - 3)}{4} \quad (53)$$

giving a maximum availability at $pH = 7$, and a minimum at $pH = 3$. If $pH < 3$ then $C_{\text{DOC,sol}} = 0$, while if $pH > 7$ then $C_{\text{DOC,sol}} = C_{\text{DOC}}$.

A5.6 Ammonia volatilisation

Ammonium is lost from the soil by volatilisation in three different processes: ammonium is lost from manure, from ammonium added in fertilisers, and from ammonium sulphate applied as fertiliser.

A5.6.1 Volatilisation loss from applied manure

Ammonium is lost from applied manure, $N_{\text{v,fym}}$ (in $\text{kg N ha}^{-1} \text{ timestep}^{-1}$), depending on the proportion of ammonium in the manure, $p_{\text{NH}_4,\text{fym}}$, the weight of manure added, W_{fym} (t ha^{-1}) and a dimensionless volatilisation quotient, $Q_{\text{v,fym}}$,

$$\text{if } R < R_{\text{crit,v}}, \text{ then } N_{\text{v,fym}} = Q_{\text{v,fym}} \times p_{\text{NH}_4,\text{fym}} \times W_{\text{fym}} \quad (54)$$

where R is the amount of rainfall (mm timestep^{-1}) and $R_{\text{crit,v}}$ is the critical level of rainfall (mm timestep^{-1}) below which volatilisation starts.

The parameters, $p_{\text{NH}_4,\text{fym}}$ and $Q_{\text{v,fym}}$ are set for each manure type. Parameters for some sample manure types are derived from the values given in table 4. The value of $Q_{\text{v,fym}}$ is set to 0.15 for all manure types.

Table 4.Parameters used to describe organic manures in ECOSSE

Manure Type	Dry matter in fresh manure (t dry weight (t fresh man.) ⁻¹)	N in dry matter in manure (kg N (t dry matter) ⁻¹)	C in dry matter in manure (kg C (t dry matter) ⁻¹)	N in manure that is NH ₄ ⁺ (%)	Percent of manure that is lost as gas (%)	Critical level of rainfall below which volatilisation occurs	N in manure that is decomposed organic matter (%)	Percent of manure added in top 25cm (%)	Liquid? (0=no; 1=yes)
Cattle FYM	25	2.4	21	20	25	5	10	100	0
Pig FYM	25	2.8	25	20	25	5	10	100	0
Layer Manure	30	5.0	32	50	30	5	25	100	0
Broiler/Turkey Manure	60	4.8	30	50	30	5	35	100	0
Sewage Sludge Cake (Undigested)	25	3.0	25	20	25	5	35	100	0
Sewage Sludge Cake (Digested)	25	3.0	25	15	25	5	35	100	0
Dairy Slurry	6	5.0	20	57	40	5	20	80	1
Beef Slurry	6	3.8	20	50	40	5	20	80	1
Pig Slurry	6	8.3	25	70	42	5	32	80	1
Strainer Box Separated Slurry	1.5	10.0	30	50	20	5	20	80	1
Weeping Wall Separated Slurry	3	10.0	30	50	20	5	25	80	1
Mechanically Separated Slurry	4	10.0	30	50	20	5	20	80	1
Sewage Sludge Liquid (Undigested)	5	3.6	25	45	40	5	15	80	1
Sewage Sludge Liquid (Digested)	4	5.0	30	45	40	5	15	80	1

A5.6.2 Volatilisation loss from fertiliser

Ammonium is volatilised from urea and ammonium sulphate added as fertiliser as calculated by the following equation:

$$\text{if } R < R_{\text{crit},v}, \text{ then } N_{v,\text{fert}} = (Q_{v,\text{urea}} \times p_{\text{urea},\text{fert}} \times N_{\text{fert}}) + (Q_{v,\text{as}} \times p_{\text{as},\text{fert}} \times N_{\text{fert}}) \quad (55)$$

where $Q_{v,\text{urea}}$ and $Q_{v,\text{as}}$ are the volatilisation quotients for urea and ammonium sulphate, set to 0.15 for both, $p_{\text{urea},\text{fert}}$ is the proportion of urea in the fertiliser, $p_{\text{as},\text{fert}}$ is the proportion of ammonium sulphate in the fertiliser, and N_{fert} is the amount of fertiliser N applied ($\text{kg N ha}^{-1} \text{ timestep}^{-1}$).

A5.7 Crop nitrogen uptake

Nitrogen is taken up by the growing plant and C and N are returned to the soil by the plant following the approach published by Bradbury et al (1993). The site specific version of the model requires detailed information about management and is designed to be used with arable crops. ECOSSE has been further developed to allow simulations when only limited data are available to describe the growing conditions of the plants.

A5.7.1 Plant Inputs

If provided as an input, the total plant inputs of C ($C_{in,tot}$) are assumed to be given by the net primary production. If the net primary production is entered as zero, the plant inputs are either calculated from the initialisation described in A2.2 or estimated using the MIAMI model (Leith, 1972). The N inputs from the plant to the soil ($N_{in,tot}$) are calculated using standard C:N ratios for the different land uses, $(C:N)_{LU}$

$$N_{in,tot} = (C:N)_{LU} \times C_{in,tot} \quad (56)$$

The C:N ratios of simple land use classes, arable, grassland, forestry and semi-natural are initially all set to 10.

As an alternative, in the site specific version of the model, the plant inputs of C and N can be calculated from the expected yield as described by Bradbury et al (1993). The plant input of carbon (C_{ao}) is given by

$$C_{in,tot} = C_{ao,1} \left(C_{ao,3} + C_{ao,2} \left(C_{ao,5} - \exp(C_{ao,3} \times W_{yield}) \right) \right) \quad (57)$$

where $C_{ao,1}$, $C_{ao,2}$, $C_{ao,3}$, $C_{ao,4}$ and $C_{ao,5}$ are empirical parameters, specific to each crop or plant type, and W_{yield} is the crop yield ($t\ ha^{-1}$) (moisture content used for the crop yield depends on the crop type).

The plant input of nitrogen (N_{ao}) is calculated from the amount of N taken up in above ground plant

$$N_{in,tot} = C_{ao,1} \left(C_{ao,3} + C_{ao,2} \left(C_{ao,5} - \exp(C_{ao,3} \times W_{yield}) \right) \right) \quad (58)$$

A5.7.2 Timing of Management Events

Management events are set using standard values for the different land use types. Arable crops are assumed to be sown in February and harvested in October: all other land uses are assumed to stay in the ground throughout the year. Arable and grassland are assumed to have fertiliser applied during March: no other land uses have fertiliser applications. Initially, farmyard manure is assumed not to be applied.

A.5.7.3 Fertiliser Applications

In the site specific version of the model, recorded fertiliser applications are entered by the user. In the limited data or GIS version of the model, the fertiliser applications for arable crops are assumed to meet the nitrogen requirement of the crop. This is a reasonable assumption, because if they did not, then the plant would not grow and the calculated C inputs would not have been achieved. If

fertiliser applications had exceeded the requirements of the crop, the losses by leaching and denitrification would have been greater than simulated. However, without further information on application rates, this cannot be estimated. If it is assumed that the N returned to the soil is the total N requirement less the N in the above ground parts of the plant at harvest, the total N requirement can be derived from equations used in SUNDIAL for total N requirement and N in above ground plant at harvest (Smith et al, 1996). Here, a typical arable crop has been taken to be a winter wheat crop with a yield of 8 t ha⁻¹ ($W_{\text{yield}} = 8$). This is a good assumption for UK conditions, but can be changed if a land use class is being derived for a differently yielding crop or for a country where winter wheat is not the dominant arable crop. The total N input to the soil as crop debris ($N_{\text{in,tot}}$) is given in SUNDIAL by

$$N_{\text{in,tot}} = (p_{\text{in,AG}} \times N_{\text{req,AG}}) + (p_{\text{in,UG}} \times N_{\text{req,UG}}) \quad (59)$$

where $p_{\text{in,AG}}$ is the proportion of N in above ground crop that is incorporated in the soil, $N_{\text{req,AG}}$ is the N in above ground, $p_{\text{in,UG}}$ is the proportion of N in below ground crop that is incorporated in the soil and $N_{\text{req,UG}}$ is the N in below ground parts of the plant at harvest. For winter wheat $p_{\text{in,AG}}$ is set to 0.12 and $p_{\text{in,UG}}$ is set to 1.0

The N in below ground parts of the plant at harvest ($N_{\text{req,UG}}$) are given by

$$N_{\text{req,UG}} = U_{r,1} \times (U_{r,3} - \exp(U_{r,2} \times W_{\text{yield}})) \quad (60)$$

where $U_{r,1}$, $U_{r,2}$ and $U_{r,3}$ are empirical parameters describing the uptake of N in below ground parts of the plant. For winter wheat, $U_{r,1} = 63$, $U_{r,2} = -0.65$ and $U_{r,3} = 1$, so $N_{\text{req,UG}} \approx 63 \text{ kg N ha}^{-1}$.

The N in above ground parts of the plant at harvest ($N_{\text{req,AG}}$) are given by

$$N_{\text{req,AG}} = U_{t,1} \times (\exp(U_{t,2} \times W_{\text{yield}}) - U_{t,3}) \quad (61)$$

where $U_{t,1}$, $U_{t,2}$ and $U_{t,3}$ are empirical parameters describing the uptake of N in below ground parts of the plant. For winter wheat, $U_{t,1} = 236$, $U_{t,2} = 0.07$ and $U_{t,3} = 1$, so $N_{\text{req,AG}} \approx 177 \text{ kg N ha}^{-1}$.

This then allows the total N requirement to be calculated from the N in the debris as

$$N_{\text{req,tot}} = \frac{N_{\text{req,tot}}}{N_{\text{in,tot}}} \times N_{\text{in,tot}} = \frac{N_{\text{in,tot}} + 0.88 \times N_{\text{req,AG}}}{N_{\text{in,tot}}} \times N_{\text{in,tot}} = \frac{63 + 177}{63} \times N_{\text{in,tot}} \approx 3.5 \times N_{\text{in,tot}} \quad (62)$$

Fertiliser requirements for grassland are estimated similarly, and for other land uses are assumed to be zero.

A.5.7.4 Pattern of Debris Incorporation

For arable crops, debris that is incorporated at harvest ($N_{\text{in,harv}}$) is calculated using the SUNDIAL parameters for winter wheat (Bradbury et al. 1993) as

$$N_{\text{in,harv}} = 0.12 \times N_{\text{in,tot}} \quad (63)$$

It is assumed that for arable crops, all other material (such as straw) is removed from the field. For other land uses, all debris is returned to the soil during the growing season as it is assumed that the plants are not harvested.

For all land use types, the pattern of carbon and nitrogen debris return during the growing season ($C_{in,preharv}$ and $N_{in,preharv}$) are assumed to follow a standard exponential relationship, as originally derived by Bradbury et al (1993) for winter wheat:

$$N_{in,preharv} = (N_{in,tot} - N_{in,harv}) \times \exp(k_{N,in} \times w) \quad (64)$$

$$C_{in,preharv} = (C_{in,tot} - C_{in,harv}) \times \exp(k_{C,in} \times w) \quad (65)$$

where w = weeks till harvest, $k_{C,in}$ is a rate constant for the incorporation of C in debris before harvest, and $k_{N,in}$ is a rate constant for the incorporation of N in debris before harvest. For winter wheat, $k_{C,in} = -0.15$ and $k_{N,in} = -0.01$. The land use types differ in the distribution and timing of C to N returned to the soil as shown in table 5.

The amount of carbon returned to the soil at harvest is given from the amount of C in stubble ($C_{in,stubble}$) and the amount of C in the straw ($C_{in,straw}$).

$$C_{in,stubble} = c_{st,1} \left(c_{st,4} - c_{st,2} \times \exp(c_{st,3} \times W_{yield}) \right) \quad (66)$$

where $c_{st,1}$, $c_{st,2}$, $c_{st,3}$, and $c_{st,4}$ are empirical parameters describing C in stubble. For winter wheat $c_{st,1} = 1446$, $c_{st,2} = 0.94$, $c_{st,3} = -0.175$ and $c_{st,4} = 1$.

$$C_{in,straw} = c_{straw,3} \times \left(c_{straw,2} \times W_{yield} \times \left(\left(1/c_{straw,1} \right) - 1 \right) \right) \quad (67)$$

where $c_{straw,1}$ is the harvest index, which for winter wheat is 0.45, $c_{straw,2}$ is the dry matter content of the straw (t dry matter / t straw), $c_{straw,3}$ is the C : dry matter ratio of the straw, and $c_{straw,4}$ (kg C / t straw dry matter). Nitrogen in straw ($N_{in,straw}$) is calculated from C using the N : dry matter ratio of the straw, $c_{straw,4}$ (kg N / t straw dry matter)

$$N_{in,straw} = c_{straw,4} \times \left(c_{straw,2} \times W_{yield} \times \left(\left(1/c_{straw,1} \right) - 1 \right) \right) \quad (68)$$

Table 5. Pattern of carbon and nitrogen inputs to the soil from land use categories, arable, grassland, forestry and semi-natural

Depth (cm)	Plant inputs in each month (kg C ha ⁻¹ month ⁻¹)											
	1	2	3	4	5	6	7	8	9	10	11	12
Arable												
0-30	0	0	0.3	0.3	0.3	0.6	1.87	0	0	0	0	0
30-100	0	0	0.3	0.3	0.3	0.3	1.17	0	0	0	0	0
>100	0	0	0.3	0.3	0.3	0.3	1.17	0	0	0	0	0

Depth (cm)	Plant inputs in each month (kg C ha ⁻¹ month ⁻¹)											
	1	2	3	4	5	6	7	8	9	10	11	12
Grassland												
0-30	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.89	0.25	0.25	0.25	0.25
30-100	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
>100	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Forestry												
0-30	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
30-100	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
>100	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Semi-Natural												
0-30	0.475	0.475	0.475	0.475	0.475	0.475	0.475	0.475	0.475	0.475	0.475	0.475
30-100	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0
>100	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0

A.5.7.5 Pattern of Nitrogen Uptake

The pattern of nitrogen uptake (N_{up}) is assumed to follow a standard pattern of nitrogen uptake for all land use types, dependent on the total N requirement for the given land use. This pattern was originally estimated using experimental data for winter wheat (Bradbury et al, 1993) as the sigmoid relationship given below:

$$N_{up} = \left(N_{req,tot}^{-1/u_1} + \exp(u_2 \times T_{sum}) \right)^{-u_1} \quad (69)$$

where $N_{req,tot}$ is the total plant N requirement (kg N ha⁻¹ year⁻¹), T_{sum} is the cumulative air temperature (°C days), and u_1 and u_2 are empirical parameters describing the sigmoid uptake of N, which for winter wheat are set to 1.5 and -0.003 respectively.

A5.8 Senescence

Nitrogen is lost from the plant by senescence following the approach published by Bradbury et al (1993).

A5.9 Evaluation of ECOSSE simulations of nitrogen transformations

An evaluation of the ECOSSE simulations of the different nitrogen transformations has been completed for a range of soil conditions, in a number of different soil environments and under different land uses. This work is currently being prepared for publication and so cannot be included here. When published, a summary of the evaluation and a reference to the published paper will be provided.

A6 Water Movement

A6.1 Vertical water movement

Vertical water movement is simulated by simple piston flow as described by (Bradbury et al. 1993).

A6.2 Restricted flow

ECOSSE uses the minimum observed depth of the water table, and the available water at saturation ($\text{mm } 5\text{cm}^{-1}$ layer), together with the long-term average monthly weather data to calculate the restriction in drainage that is required to achieved the minimum water table depth observed. If there is no restriction to drainage, within a few hours of a rainfall event, it can be assumed that water drained (D_u) can be calculated from rainfall (R) and potential evapotranspiration (E_T) as

$$D_u = R - E_T \quad (70)$$

However, if water flow through the soil profile is restricted then drainage is reduced. Under restricted drainage conditions, water drained (D_r) is reduced by the amount of water building up in the profile rather than draining,

$$D_r = R - E_T - \sum_i^n (\psi_s - \psi_f) \quad (71)$$

where ψ_s is the available water at saturation and ψ_f is the available water at field capacity for layer i , where i ranges between the layer at the minimum depth of the water table, and n is deepest layer in the profile. The restriction in drainage at a particular site (p_r) can then be expressed as the ratio of water drained in restricted and unrestricted conditions

$$p_r = \frac{D_r}{D_u} = \frac{R - E_T - \sum_i^n (\psi_s - \psi_f)}{R - E_T} \quad (72)$$

It is assumed that the restriction in drainage is due to a general characteristic of the soil profile, rather than a restriction at one point in the profile (such as an impermeable layer). Therefore, this restriction to drainage is cumulated as excess drainage (D_{ex}) over all layers:

$$D_{ex} = \sum_{i=1}^n p_r \times D_i \quad (73)$$

where D_i is the unrestricted drainage in layer i . The excess drainage is then used to re-adjust the water content of the layers from the bottom of the profile upwards, so simulating at the equilibrium point at the start of the simulation, saturated layers below the observed depth of water table. This restriction to drainage is then used throughout the simulation to calculate the changes in water table depth following rainfall and evapotranspiration.

A6.3 Evaluation of ECOSSE simulations of water movement

An evaluation of the ECOSSE simulations of the water movement has been completed for a range of soil conditions, in a number of different soil environments and under different land uses. This work is currently being prepared for publication and so cannot be included here. When published, a summary of the evaluation and a reference to the published paper will be provided.

PART B - SITE SPECIFIC SIMULATIONS

B1 Input files

The formats of the input files for the site specific version are complex as they were originally designed to be accessed via a DOS based graphical user interface, and not directly by the user. However, with the development of the Windows operating system, the DOS interface is now obsolete, and so users more often access the files directly using an editor. If you would like a copy of the DOS-based graphical user interface, please contact the authors.

B1.1 Management Data

B1.1.1 Input through file MANAGEMENT.DAT

If file MANAGEMENT.DAT exists, this file will provide management data.

Format of example file is shown below. Data value is entered in the first 10 spaces of each line. The

2	Soil code number
2	Drainage class (1=low; 2=moderate; 3=high)
1	Depth to impermeable layer (1=50cm; 2=100cm; 3=150cm)
1	Previous crop (code given in CROP_SUN.DAT)
7	Yield of previous crop (t / ha)
35	Atmospheric N deposition (kg N / ha)
1	Date field reaches field capacity (1=01/01; 2=01/06)
1	Timestep (0 = 30 minute; 1 = daily; 2 = weekly; 3 = monthly)
0	Crop model type (0=SUNDIAL; 1=MAGEC)
10	Number of years included in the simulation
243	Timesteps from 01/01/01 to harvest of previous crop
2003	First year of simulation
3650	End of simulation
0	Fixed end of simulation (0=No; 1=Yes)
53	Latitude
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
' daily.dy '	Met.file year 1
9	Number of crops
6	CROP 1: Crop code (code given in CROP_SUN.DAT)
273	Timesteps to sowing date from 01/01/01
0	Crop N uptake at harvest (0 = calculate internally) kg N / ha
623	Timesteps to harvest date from 01/01/01
5	Expected yield (t/ha)
0	Crop residues incorporated (0=No; 1=Yes)
1	Number of fertiliser application
0	Number of manure applications
200	CROP 1, FERT 1: Amount of fertiliser applied (kg N / ha)
455	Timesteps to application date from 01/01/01
100	% Nitrate
0	% Non-urea N
0	% Urea N
0	Does fertiliser contain ammonium salts other than ammonium sulphate? (0=No; 1=Yes)
0	Is fertiliser labelled?

explanatory note on each line is not read by the model.

B1.1.2 Input by setup file

If MANAGEMENT.DAT does not exist, management is read in from SETUP file. The name of the SETUP file is read in from FNames.DAT. Name of file is held within speech marks. The format of FNames.DAT shown below.

Line 1: 'sbarley.set'

The format of the SETUP file is as given below. The top cells on each line shows the values entered in the file in free format, space separated. The text in the lower cells indicates the meaning of each item. Additional crops are added by repeating the lines shown for crop 1. Empty cells are omitted from the file.

Input variable	Soil Type (SOIL_PARS.DAT)	Drainage class	Depth to impermeable layer	Previous crop code (PARLIS.OUT)	Previous crop yield (t/ha)	Period under grass in the past 10 years (not changed)	Atmospheric N deposition (kg N / ha)	Date field reaches field capacity (1=01/01; 2=01/06)
Line 1	12 "Waite"	2 Moderate	2 100cm	6 Spring Barley	5.53	1 None	0 Error! Too low!	1 1-Jan

Input variable	Number of years included in the simulation	Date of first harvest	First year in simulation	Start of simulation (not changed)	End of simulation (not changed)	Fixed end to simulation? (0=No, 1=Yes)	Latitude
Line 2	5	232 22-Aug-88	1988	1	1830 Error! Too high!	0 No	50

Input variable	Weather File		
Line 3	'	eisen88.dy	'
Line 4	'	eisen89.dy	'
Line 5	'		'
Line 6	'		'
Line 7	'		'
Line 8	'		'
Line 9	'		'
Line 10	'		'
Line 11	'		'
Line 12	'		'

Input variable	Number of crops
Line 13	1

CROP 1 Input variable	Crop code (PARLIS.OUT)	Sowing date	Crop N uptake at harvest (0 = calculate internally)	Harvest date	Expected yield (t/ha)	Crop residues incorporated (0=No, 1=Yes)	Number of fertiliser applications	Number of organic manure applications
Line 14	9 Maincrop Potatoes	457 5-Apr-1989	0 Calculate internally	665 30-Oct-1989	43.91	0 No	4	0

CROP 1 FERTILISERS Input variable	Amount of fertiliser N applied (kg N / ha)	Timesteps to application date from 01/01/01	% Nitrate N	% Non-Urea N	% Urea N	Does fertiliser contain ammonium salts other than ammonium sulphate? (0=No; 1=Yes)	Is fertiliser labelled? (0=No; 1=Yes)
Line 15	36	453 1-Apr-1989	0	100	0	1 Yes	0 No
Line 16	63	477 25-Apr-1989	0	100	0	0 No	0 No
Line 17	14	498 16-May-1989	25	25	50	1 Yes	0 No
Line 18	46	501 19-May-1989	0	0	100	1 Yes	0 No
Line 19							

CROP 1 MANURES Input variable	Amount of organic manure applied (t manure fresh weight / ha)	Timesteps to application date from 01/01/01	Manure type	Is manure labelled? (0=No; 1=Yes)
Line 20				
Line 21				
Line 22				
Line 23				
Line 24				

This example file is shown as it appears below.

12	2	2	6	5.53	1	0	1	1	0
5	232	1988	1	1830	0	50			
'eisen88.dy'		0							
'eisen89.dy'		0							
1									
9	457	0	665	43.91	0	4	0		
36	453	0	100	0	1	0			
63	477	0	100	0	0	0			
14	498	25	25	50	1	0			
46	501	0	0	100	1	0			

B1.2. Weather Data

Weather data is entered in files specified in management files. Note column titles are not included in the input files. Data is entered as space separated values.

	Timestep number	SUNDIAL Crop Model			MAGEC Crop Model Only				
		Rainfall (mm timestep ⁻¹)	Potential Evapotranspiration over Grass (mm timestep ⁻¹)	Average air temperature (°C)	Daily global radiation (J m ⁻² ground d ⁻¹)	Daily minimum temperature (°C)	Daily maximum temperature (°C)	Vapour pressure (kPa)	Daily wind speed (m s ⁻¹)
Line 1	1	10.9	0.2	1.9	2400000	-1.3	5.1	0.55	1.96
Line 2	2	5.5	-0.6	3.05	2000000	-0.8	6.9	0.87	3.08
...	3	0	0.2		3000000	0.9	3.1	0.5	2.8
....	364	5.5	-0.2	9.25	600000	8	10.5	1.17	6.76
Line 365	365	9.3	0.5	7.95	1600000	6.4	9.5	0.91	3.43

This example file is shown as it appears below.

1	10.9	0.2	1.9	2400000	-1.3	5.1	0.55	1.96
2	5.5	-0.6	3.05	2000000	-0.8	6.9	0.87	3.08
3	0	0.2	2	3000000	0.9	3.1	0.5	2.8
4	6.1	0.2	-0.1	2500000	-4.6	4.4	0.41	1.85
5	0.2	-0.5	-0.85	1000000	-3.8	2.1	0.66	3.34
6	0	0	0.55	2400000	-0.4	1.5	0.59	1.84
7	15.3	0.3	-1.4	1100000	-4	1.2	0.47	4.78
8	3.4	-0.1	0.2	900000	-0.6	1	0.62	1.67
9	4.2	0.6	3.8	2100000	0.1	7.5	0.64	2.5
10	2.3	-0.6	5.8	1300000	0.2	11.4	1.01	4.21
11	0	0.4	5.2	3300000	2.6	7.8	0.71	5.69
12	0	1.2	6.1	3500000	2.9	9.3	0.59	5.2
13	0	0.2	7.15	800000	3.3	11	0.95	7.35
14	0.2	0	6.15	3100000	5.3	7	0.88	7.5
15	0.3	0.5	4.65	1900000	3.6	5.7	0.69	3.74
16	0	0	1.35	3900000	-0.3	3	0.51	1.15
17	2.2	0.8	3.45	2800000	-2.6	9.5	0.57	2.4
18	0.5	-1.1	5.2	2100000	-0.3	10.7	1.13	4.79
19	4.2	0.4	9.9	1100000	9.2	10.6	1.1	5.93
20	3.1	0.6	4.4	3900000	0.9	7.9	0.63	5.12
21	0	-0.3	5.3	3600000	2.2	8.4	0.89	3.48
22	5.5	0.5	4.9	800000	0.6	9.2	0.73	5.08

B1.3 Crop Parameters

Crop parameters are entered through file CROP_SUN.DAT. The format of the file is as shown below:

Line 1: Crop name

Line 2: Crop code number

Line 3: Parameters describing total C in crop debris: $C_{ao,1}$, $C_{ao,2}$, $C_{ao,3}$, $C_{ao,4}$ and $C_{ao,5}$, as defined in section A 5.7.1.

Line 4: Parameters describing uptake of N in below ground parts of the plant, $U_{r,1}$, $U_{r,2}$, $U_{r,3}$; and parameters describing uptake of N in above ground parts of the plant, $U_{t,1}$, $U_{t,2}$, $U_{t,3}$, as defined in section A 5.7.3.

Line 5: Parameters describing the proportions of N in above and below ground crop that are incorporated in the soil, $p_{in,AG}$ and $p_{in,UG}$ respectively as described in section A 5.7.3. Rate constants for incorporation of C and N in debris before harvest, as described in section A 5.7.4.

Line 6: Fraction of N taken up by the crop that is senesced after anthesis, amount of N in seed (kg N ha^{-1}), Empirical parameters describing uptake of N by the crop, u_1 and u_2 , respectively, as described in section A 5.7.5.

Line 7: Period of senescence (weeks); rate of root growth (cm week^{-1}); depth above current root depth from which N extraction can occur (cm); maximum rooting depth (cm).

Line 8: Empirical parameters describing C in the stubble (non-cartable crop debris), $c_{st,1}$, $c_{st,2}$, $c_{st,3}$, and $c_{st,4}$ as described in section A 5.7.4.

Line 9: Parameters describing C and N in straw as described in section A 5.7.4; $c_{straw,1}$ the harvest index, $c_{straw,2}$ the dry matter content of the straw (t dry matter / t straw), $c_{straw,3}$ the C : dry matter ratio of the straw, and $c_{straw,4}$ the N : dry matter ratio of the straw ($\text{kg N} / \text{t straw dry matter}$).

B1.4 Soil Parameters

If file SOIL.DAT exists, the soil parameters are read in through this file.

The format of example file is shown below. Data value is entered in the first 9 spaces of each

Peat Soil	
2	Soil code number (used in management file)
45	Available water (mm / 0-25cm)
0.118	Stable N:C ratio of biomass and humus
0.29	Fraction (biomass+humus)/(Total decomposition)
1.1	Biomass/Humus produced from biomass decomposition
1.1	Biomass/Humus produced from humus decomposition
0.028	Fraction of biomass in total organic C
10	Minimum level of nitrate in soil (kg N / ha / 50cm layer)
0.66	Rate constant for biomass decomposition (/year)
0.02	Rate constant for humus decomposition (/year)
150000	Total organic matter in top 50cm of soil (kg C / ha)
27061	Inert organic matter in top 50cm of soil (kg C / ha)
4	Land use before equilibrium run (1=arable; 2=grass; 3=forestry; 4=natural/scrub)
1	Land use after equilibrium run but before start of simulation proper (1=arable; 2=grass; 3=forestry; 4=natural/scrub)
100	Number of years between equilibrium and start of simulation proper
'ppt1900-2000.dat'	File containing monthly rain for the period between equilibrium and start of simulation. Format: Rainfall (mm) Y
'temp1900-2000.dat'	File containing monthly temp for the period between equilibrium and start of simulation. Format: Temperature (C) Y
'pet1900-2000.dat'	File containing monthly potential open pan evapotranspiration for the period between equilibrium and start of simulation. Format: PET (mm) Y
1	% Clay content
25	Depth of soil used in initialisation
6.5	pH of soil
2.5	pH at which decomposition has declined to zero
5.5	pH at which decomposition starts to decline

line.

The explanatory note on each line is not read by the model.

If file SOIL.DAT does not exist, soil parameters are entered through file SOIL_PAR.DAT.

Soil Name	Soil Number	Stable N:C ratio of biomass & humus pools	Organic C (kg C / ha)	Organic matter modifier for grass	Fraction of BIO + HUM formed (alpha+beta)	Propn. BIO:HUM (alpha:beta) from BIO	Propn. BIO:HUM (alpha:beta) from HUM	Fraction of BIO in total organic C and N	Minimum level of nitrate in soil (kg N / ha / 50cm layer)	Rate constant for biomass decomposition (/ year)	Rate constant for humus decomposition (/ year)	Total organic matter in top 50cm of soil (kg C / ha)	Inert organic matter content of soil type (kg C / ha)	Land use history (1=arable, 2=grassland, 3=forestry)	% Clay content	Depth of soil used in initialisation	pH of soil	which decomposition has	decomposition starts to decline
Peat Soil	155	0.118	82039	1	0.29	1.1	1.1	0.028	10	0.66	0.02	150000	27061	4	1	25	6.5	2.5	5.5

B1.5 Water table depth

If the water table depth has been measured and should be used as an input by the model, the data should be entered in file "WTD.DAT", in the following format.

Line 1, end:

Number of timestep from beginning of simulation when water table depth is measured
Depth of water table (cm)

B2 Output files

PART C - LIMITED DATA SITE SIMULATIONS

C1 Input files

C1.1 Site and management data

New Line: Mode of equilibrium run: calculate C pools...

- 1=using known PI
- 2= adjusting PI to give measured TOC
- 3=adjusting decomp.rate to give meas.PI and TOC
- 4=using C accumulation
- 5=using fixed proportions of C pools
- 6=using TOC and the Hillier solver (analytical soln of RothC =brium run)
to get PI & C pools
- 7= adjusting PI to give measured TOC, and further adjusting PI during
dynamic phase of the simulation according to current weather

New Line: n = Number of layers (max. 10)

New Line: Depth of top of SOM layer 1 (cm)

New Line: Depth of top of SOM layer 2 (cm)

New Line: ...Depth of top of SOM layer n (cm)

For this soil under arable:

In SOM layer 1

New Line: C content (kg C / ha)

New Line: Bulk density (g/cm³)

New Line: Soil pH

New Line: % clay by weight

New Line: % silt by weight

New Line: % sand weight

In SOM layer 2...

In SOM layer n...

For this soil under grassland:

In SOM layer 1

New Line: C content (kg C / ha)

New Line: Bulk density (g/cm³)

New Line: Soil pH

New Line: % clay by weight

New Line: % silt by weight

New Line: % sand weight

In SOM layer 2...

In SOM layer n...

For this soil under forestry:

In SOM layer 1

New Line: C content (kg C / ha)

New Line: Bulk density (g/cm³)

New Line: Soil pH

New Line: % clay by weight

New Line: % silt by weight

New Line: % sand weight

In SOM layer 2...

In SOM layer n...

For this soil under natural/seminatural:

In SOM layer 1

New Line: C content (kg C / ha)

New Line: Bulk density (g/cm³)

New Line: Soil pH

New Line: % clay by weight

New Line: % silt by weight
 New Line: % sand weight
 In SOM layer 2...
 In SOM layer n...
 New Line: Arable long term average plant C input (kg C /ha/yr) (used in modes 1 & 3 only)
 New Line: Grassland long term average plant C input (kg C /ha/yr) (used in modes 1 & 3 only)
 New Line: Forestry long term average plant C input (kg C /ha/yr) (used in modes 1 & 3 only)

New Line: Natural long term average plant C input (kg C /ha/yr) (used in modes 1 & 3 only)
 Long term average rainfall (mm/month)
 New Line: January
 New Line: February
 New Line: March
 New Line: April
 New Line: May
 New Line: June
 New Line: July
 New Line: August
 New Line: September
 New Line: October
 New Line: November
 New Line: December
 Long term average temperature (deg.C/month)
 New Line: January
 New Line: February
 New Line: March
 New Line: April
 New Line: May
 New Line: June
 New Line: July
 New Line: August
 New Line: September
 New Line: October
 New Line: November
 New Line: December
 New Line: Latitude
 New Line: Water table depth at start (cm)
 New Line: Drainage class (Not yet used)
 New Line: C accum.before change (kgC/ha/yr) (only in mode 4 – if not dummy value)
 New Line: CH4 emission before change (kgC/ha/yr) (not used yet)
 New Line: CO2 emission before change (kgC/ha/yr) (not used yet)
 New Line: DOC loss before change (kgC/ha/yr) (not used yet)
 New Line: Number of growing seasons, g
 New Line x g: For each growing season: Land use, plant input (kg C / ha / yr) – (not used in mode 7 -
 if plant input not given, unused and plant input obtained from RothC instead)
 1=arable
 2=grassland
 3=forestry
 4=natural/seminatural
 New Line x g: Name of annual weather file (if used). If not given use long term average. (Format:
 Month,Rain(mm/mon),PET(mm/mon),Temp(deg.C/mon)) Note: need quotes round file name

Example file:

2 Mode of run
 3 Number of layers
 18 Depth of bottom of SOM layer 1 (cm)
 68 Depth of bottom of SOM layer 2 (cm)
 80 Depth of bottom of SOM layer 3 (cm)
 196946 C content (kg C / ha) - for this soil under arable in SOM layer 1

0.34 Bulk density (g/cm³) - for this soil under arable in SOM layer 1
 5.95 pH - for this soil under arable in SOM layer 1
 7 % clay by weight - for this soil under arable in SOM layer 1
 23 % silt by weight - for this soil under arable in SOM layer 1
 70 % sand by weight - for this soil under arable in SOM layer 1
 16462 C content (kg C / ha) - for this soil under arable in SOM layer 2
 1.49 Bulk density (g/cm³) - for this soil under arable in SOM layer 2
 5.91 pH - for this soil under arable in SOM layer 2
 9 % clay by weight - for this soil under arable in SOM layer 2
 21 % silt by weight - for this soil under arable in SOM layer 2
 70 % sand by weight - for this soil under arable in SOM layer 2
 7280 C content (kg C / ha) - for this soil under arable in SOM layer 3
 1.52 Bulk density (g/cm³) - for this soil under arable in SOM layer 3
 5.42 pH - for this soil under arable in SOM layer 3
 12 % clay by weight - for this soil under arable in SOM layer 3
 18 % silt by weight - for this soil under arable in SOM layer 3
 70 % sand by weight - for this soil under arable in SOM layer 3
 3 pH - for this soil under grassland in SOM layer 1
 33 % clay by weight - for this soil under grassland in SOM layer 1
 33 % silt by weight - for this soil under grassland in SOM layer 1
 34 % sand by weight - for this soil under grassland in SOM layer 1
 33 % silt by weight - for this soil under grassland in SOM layer 1
 34 % sand by weight - for this soil under grassland in SOM layer 1
 0 C content (kg C / ha) - for this soil under grassland in SOM layer 2
 1.3 Bulk density (g/cm³) - for this soil under grassland in SOM layer 2
 3 pH - for this soil under grassland in SOM layer 2
 33 % clay by weight - for this soil under grassland in SOM layer 2
 33 % silt by weight - for this soil under grassland in SOM layer 2
 34 % sand by weight - for this soil under grassland in SOM layer 2
 0 C content (kg C / ha) - for this soil under grassland in SOM layer 3
 1.3 Bulk density (g/cm³) - for this soil under grassland in SOM layer 3
 3 pH - for this soil under grassland in SOM layer 3
 33 % clay by weight - for this soil under grassland in SOM layer 3
 33 % silt by weight - for this soil under grassland in SOM layer 3
 34 % sand by weight - for this soil under grassland in SOM layer 3
 45100 C content (kg C / ha) - for this soil under forestry SOM layer 1
 1.3 Bulk density (g/cm³) - for this soil under forestry in SOM layer 1
 3 pH - for this soil under forestry in SOM layer 1
 33 % clay by weight - for this soil under forestry in SOM layer 1
 33 % silt by weight - for this soil under forestry in SOM layer 1
 34 % sand by weight - for this soil under forestry in SOM layer 1
 0 C content (kg C / ha) - for this soil under forestry SOM layer 2
 1.3 Bulk density (g/cm³) - for this soil under forestry in SOM layer 2
 3 pH - for this soil under forestry in SOM layer 2
 33 % clay by weight - for this soil under forestry in SOM layer 2
 33 % silt by weight - for this soil under forestry in SOM layer 2
 34 % sand by weight - for this soil under forestry in SOM layer 2
 0 C content (kg C / ha) - for this soil under forestry SOM layer 3
 1.3 Bulk density (g/cm³) - for this soil under forestry in SOM layer 3
 3 pH - for this soil under forestry in SOM layer 3
 33 % clay by weight - for this soil under forestry in SOM layer 3
 33 % silt by weight - for this soil under forestry in SOM layer 3
 34 % sand by weight - for this soil under forestry in SOM layer 3
 196946 C content (kg C / ha) - for this soil under semi-natural / natural in SOM layer 1
 0.34 Bulk density (g/cm³) - for this soil under semi-natural / natural in SOM layer 1
 3.34 pH - for this soil under semi-natural / natural in SOM layer 1
 0 % clay by weight - for this soil under semi-natural / natural in SOM layer 1
 0 % silt by weight - for this soil under semi-natural / natural in SOM layer 1
 0 % sand by weight - for this soil under semi-natural / natural in SOM layer 1
 458584 C content (kg C / ha) - for this soil under semi-natural / natural in SOM layer 2

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'NH200600_1980.dat' Weather files to be used in dynamic simulations 'NH200600_1981.dat'
'NH200600_1982.dat'
'NH200600_1983.dat'
'NH200600_1984.dat'
'NH200600_1985.dat'
'NH200600_1986.dat'
'NH200600_1987.dat'
'NH200600_1988.dat'
'NH200600_1989.dat'
'NH200600_1990.dat'
'NH200600_1991.dat'
'NH200600_1992.dat'
'NH200600_1993.dat'
'NH200600_1994.dat'
'NH200600_1995.dat'
'NH200600_1996.dat'
'NH200600_1997.dat'
'NH200600_1998.dat'
'NH200600_1999.dat'
'NH200600_2000.dat'
'NH200600_2001.dat'
'NH200600_2002.dat'
'NH200600_2003.dat'
'NH200600_2004.dat'
'NH200600_2005.dat'

C1.2 Weather data

Note: no title line!

Line 1-12: In free format with no commas: Month number (1-12), rainfall (mm/month), potential evapotranspiration (mm/month) and air temperature (°C).

C2 Output files

PART D - SPATIAL SIMULATIONS

D1 Input files

The GIS simulations are driven through input files, that are supplied in the control file, G NAMES.DAT, which contains the names of all other files used in the simulation.

D1.1 File G NAMES.DAT

Line 1: Name of input file containing NPP and soil information

Line 2: Name of input file containing LU information

For non-SSKIB run

Line 3: Name of file containing soil codes

Lines 4-6 = blank

For SSKIB run = names of files containing

Line 3: 1. soil codes under arable;

Line 4: 2. soil codes under grassland;

Line 5: 3. soil codes under forestry;

Line 6: 4. soil codes under nat/semi-nat;

Line 7: 5. soil codes under miscanthis;

Line 8: 6. soil codes under SRC.

Line 9: Name of output file for results on 1km² grid

Line 10: Name of output file for results on 20km² grid

Line 11: Name of output file for results on 1km² grid organic soil

Line 12: Name of output file for results on 20km² grid organic soil

Line 13: Depth of reporting (cm)

For Scottish data non-SSKIB and SSKIB climate change runs

Line 14: Name of future climate file (if looking at climate change – if not just miss off)

For JULES climate change run

Line 15a: Name of future rainfall file (if looking at climate change – if not just miss off)

Line 15b: Name of future temperature file (if looking at climate change – if not just miss off)

Line 15c: Name of future NPP file (if looking at climate change – if not just miss off)

For all climate change runs

Line 16: Name of climate change results file (if looking at climate change – if not just miss off)

Line 17: Name of climate change organic results file (if looking at climate change – if not just miss off)

D1.2 Input File for NPP and Soil Information

Line 1: Title line

Line 2 to end: Grid ID (20km²)
Grid ID (1km²)
Eastings coordinate (m)
Northings (m)
Area of 1km² grid occupied by land (m²)
Dominant soil series 1
Percentage of cell under dominant soil series 1
Soil wetness class series 1
Dominant soil series 2
Percentage of cell under dominant soil series 2
Soil wetness class series 2

Dominant soil series 3
 Percentage of cell under dominant soil series 3
 Soil wetness class series 3
 Dominant soil series 4
 Percentage of cell under dominant soil series 4
 Soil wetness class series 4
 Dominant soil series 5
 Percentage of cell under dominant soil series 5
 Soil wetness class series 5
 Remaining percentage of cell under other soil series
 Net primary production $\text{kgC m}^{-2} \times 1000$ for this 1km^2 grid cell
 Long Term Average Rainfall (mm month^{-1}) Jan to Dec
 Long Term Average Air Temperature ($^{\circ}\text{C month}^{-1}$) Jan to Dec
 Longitude
 Latitude

D1.3 Format of Input File for LU Information

Line 1: Title line

Line 2 to end: Grid ID (20km^2)
 Grid ID (1km^2)
 Eastings coordinate (m)
 Northings (m)
 Area of 1km^2 grid occupied by land (m^2)
 Fraction of cell under arable at start
 Fraction of cell under gardens at start (not used)
 Fraction of cell under semi-natural/natural at start
 Fraction of cell under other at start (not used)
 Fraction of cell under grassland at start
 Fraction of cell under sea at start (not used)
 Fraction of cell under forestry at start
 Fraction of cell under urban at start
 Fraction of cell under water at start
 Fraction of cell under land with non-CORINE definition at start
 Fraction of cell under miscanthus at start
 Fraction of cell under SRC at start
 LU1 changed to LU2 in decade 1 ($\text{ha decade}^{-1} 20\text{km}^2$)
 LU1=Forestry; LU2=Forestry;
 LU1=Natural/Semi-natural; LU2=Forestry;
 LU1=Grassland; LU2=Forestry;
 LU1=Arable; LU2=Forestry;
 LU1=Miscanthus; LU2=Forestry;
 LU1=SRC; LU2=Forestry;
 LU1=Forestry; LU2= Natural/Semi-natural;
 LU1=Natural/Semi-natural; LU2= Natural/Semi-natural;
 LU1=Grassland; LU2= Natural/Semi-natural;
 LU1=Arable; LU2= Natural/Semi-natural;
 LU1=Miscanthus; LU2= Natural/Semi-natural;
 LU1=SRC; LU2= Natural/Semi-natural;
 LU1=Forestry; LU2=Grassland;
 LU1=Natural/Semi-natural; LU2=Grassland;
 LU1=Grassland; LU2=Grassland;
 LU1=Arable; LU2=Grassland;
 LU1=Miscanthus; LU2=Grassland;
 LU1=SRC; LU2=Grassland;
 LU1=Forestry; LU2=Arable;
 LU1=Natural/Semi-natural; LU2=Arable;
 LU1=Grassland; LU2=Arable;

LU1=Arable; LU2=Arable;
 LU1=Miscanthus; LU2=Arable;
 LU1=SRC; LU2=Arable;
 LU1=Forestry; LU2= Miscanthus;
 LU1=Natural/Semi-natural; LU2= Miscanthus;
 LU1=Grassland; LU2= Miscanthus;
 LU1=Arable; LU2= Miscanthus;
 LU1=Miscanthus; LU2= Miscanthus;
 LU1=SRC; LU2= Miscanthus;
 LU1=Forestry; LU2=SRC;
 LU1=Natural/Semi-natural; LU2=SRC;
 LU1=Grassland; LU2=SRC;
 LU1=Arable; LU2=SRC;
 LU1=Miscanthus; LU2=SRC;
 LU1=SRC; LU2=SRC.

Fraction of LU1 changed to LU2 in decade 2 (ha decade⁻¹ 20km⁻²)
 LU1=Forestry; LU2=Forestry...
 ...LU1=Other; LU2=Other.

Fraction of LU1 changed to LU2 in decade 3 (ha decade⁻¹ 20km⁻²)
 LU1=Forestry; LU2=Forestry...
 ...LU1=Other; LU2=Other.

Fraction of LU1 changed to LU2 in decade 4 (kha yr⁻¹ 20km⁻²)
 LU1=Forestry; LU2=Forestry...
 ...LU1=Other; LU2=Other.

Fraction of LU1 changed to LU2 in decade 5 (kha yr⁻¹ 20km⁻²)
 LU1=Forestry; LU2=Forestry...
 ...LU1=Other; LU2=Other.

Fraction of LU1 changed to LU2 in decade 5 (kha yr⁻¹ 20km⁻²)
 LU1=Forestry; LU2=Forestry...
 ...LU1=Other; LU2=Other.

D1.4 Format of Input File for Soil Codes

D1.4.1 Non SSKIB Data

Line 1: Title line

Line 2 to end: Series code number (match numbers used in NPP and soil information file)

For an arable soil

Layer 1 (0-30cm)

Percent carbon

Carbon content C (kg x 10⁶ km⁻²)

Percent clay

Percent silt

Percent sand

Bulk density (g cm⁻³)

Layer 2 (30-100cm)

Percent carbon...

...Bulk density (g cm⁻³)

Layer 3 (Over 100cm)

Percent carbon...

...Bulk density (g cm⁻³)

For a grassland soil

Layer 1 (0-30cm)

Percent carbon...

...Bulk density (g cm⁻³)

Layer 2 (30-100cm)

Percent carbon...

...Bulk density (g cm⁻³)
 Layer 3 (Over 100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 For a semi-natural / natural soil
 Layer 1 (0-30cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 2 (30-100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 3 (Over 100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 For a forest soil
 Layer 1 (0-30cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 2 (30-100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 3 (Over 100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 For a miscanthus soil
 Layer 1 (0-30cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 2 (30-100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 3 (Over 100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 For a SRC soil
 Layer 1 (0-30cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 2 (30-100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)
 Layer 3 (Over 100cm)
 Percent carbon...
 ...Bulk density (g cm⁻³)

D1.4.2 SSKIB Data

Note: -9999 = missing data. LU on this soil type is omitted from calculation. This provides a means of omitting unrealistic land uses (eg arable on peatland)

Arable Soil Codes File

Line 1: Title line

Line 2 to end: Series code number (match numbers used in NPP and soil information file)
 Flag for impermeable layer (0 = no impermeable/rock layer; 1 = impermeable / rock layer)
 Depth of impermeable layer (if present) (cm)

Layer 1
 Top depth (cm)
 Bottom depth (cm)
 Thickness (cm)
 pH measured in water
 Percent C
 C (kg ha⁻¹)
 Percent clay
 Percent silt
 Percent sand
 Bulk density (g cm⁻³)
 Percent stones

Layer 2
 Top depth (cm)...
 ...Percent stones

Layer 3
 Top depth (cm)...
 ...Percent stones

Layer 4
 Top depth (cm)...
 ...Percent stones

Layer 5
 Top depth (cm)...
 ...Percent stones

Layer 6
 Top depth (cm)...
 ...Percent stones

Layer 7
 Top depth (cm)...
 ...Percent stones

Layer 8
 Top depth (cm)...
 ...Percent stones

Layer 9
 Top depth (cm)...
 ...Percent stones

Soil Codes files for other land uses using the same format.

D1.5 Format of Input File for Future Climate

D1.5.1 Scottish non-SSKIB and SSKIB

For each 1km² grid cell, UKCIP data is given in the following format:

Lines 1 to end: ID of 20km² grid containing the cell,
 ID of 1km² cell,
 Easting,
 Northing,
 Average monthly temperature (°C) for Jan – Dec 2020,
 Total monthly precipitation (mm) for Jan – Dec 2020,
 Average monthly temperature (°C) for Jan – Dec 2050,
 Total monthly precipitation (mm) for Jan – Dec 2050,
 Average monthly temperature (°C) for Jan – Dec 2080,
 Total monthly precipitation (mm) for Jan – Dec 2080

D1.5.2 Format of Input File for Future Rainfall (JULES run)

For each 1km² grid cell, UKCIP data is given in the following format:

Lines 1 to end: ID of 20km² grid containing the cell,
ID of 1km² cell,
Easting,
Northing,
Total monthly precipitation (mm) for months 1-12 in years 1-90

D1.5.3 Format of Input File for Future Temperature (JULES run)

For each 1km² grid cell, UKCIP data is given in the following format:

Lines 1 to end: ID of 20km² grid containing the cell,
ID of 1km² cell,
Easting,
Northing,
Average monthly temperature (°C) for months 1-12 in years 1-90

D1.5.4 Format of Input File for Net Primary Production (JULES run)

For each 1km² grid cell, UKCIP data is given in the following format:

Lines 1 to end: ID of 20km² grid containing the cell,
ID of 1km² cell,
Easting,
Northing,
Average monthly NPP (kg C / ha / month) for months 1-12 in years 1-90 for land uses
1-4 (1=arable; 2=grassland; 3=forestry; 4=semi-natural)

D2 Output files

D2.1 Format of Output File for Results on 1km² grid

For each 1km² grid cell, results are given for the profile to the depth specified in line 9 of G NAMES.DAT

Lines 1 & 2: Title lines

Lines 3 to end: ID of 20km² grid containing the cell,
ID of 1km² cell,
Easting,
Northing,
Carbon change per land use change (kt C km⁻² 10years⁻¹)
Decade 1
Arable to arable
Grassland to arable
Forestry to arable
Natural/semi-natural to arable
Miscanthus to arable
SRC to arable

Arable to grassland
Grassland to grassland
Forestry to grassland
Natural/semi-natural to grassland
Miscanthus to grassland
SRC to grassland

Arable to forestry
Grassland to forestry
Forestry to forestry
Natural/semi-natural to forestry
Miscanthus to forestry
SRC to forestry

Arable to natural/semi-natural
Grassland to natural/semi-natural
Forestry to natural/semi-natural
Natural/semi-natural to natural/semi-natural
Miscanthus to natural/semi-natural
SRC to natural/semi-natural

Arable to miscanthus
Grassland to miscanthus
Forestry to miscanthus
Natural/semi-natural to miscanthus
Miscanthus to miscanthus
SRC to miscanthus

Arable to SRC
Grassland to SRC
Forestry to SRC
Natural/semi-natural to SRC
Miscanthus to SRC
SRC to SRC

Decade 2
Arable to arable
....

Decade 3
Arable to arable
....

Decade 4
Arable to arable
....

Decade 5
Arable to arable
....

Decade 6
Arable to arable
....

Decade 7 (LU change projections using decade 6)
Arable to arable
....

Carbon change for all soils in the cell (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Carbon change for organic soils in the cell only (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Carbon dioxide emissions for all soils in the cell (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Methane emissions for all soils in the cell (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Nitrous oxide emissions for all soils in the cell (kt N km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Total losses in CO₂ equivalents for all soils in the cell (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6
Decade 7 (LU change projections using decade 6)

Total losses in CO₂ equivalents for organic soils in the cell only (kt C km⁻² 10years⁻¹)

Decade 1
Decade 2
Decade 3
Decade 4
Decade 5
Decade 6

D2.2 Format of Output File for Results on 20km² grid

For each 20km² grid cell, results are given for the profile to the depth specified in line 9 of G NAMES.DAT

Lines 1 & 2: Title lines

Lines 3 to end: ID of 20km² grid containing the cell,
Easting,
Northing,
Carbon change per land use change (kt C km⁻² 10years⁻¹)

Decade 1

Arable to arable
Grassland to arable
Forestry to arable
Natural/semi-natural to arable
Miscanthus to arable
SRC to arable

Arable to grassland
Grassland to grassland
Forestry to grassland
Natural/semi-natural to grassland
Miscanthus to grassland
SRC to grassland

Arable to forestry
Grassland to forestry
Forestry to forestry
Natural/semi-natural to forestry
Miscanthus to forestry
SRC to forestry

Arable to natural/semi-natural
Grassland to natural/semi-natural
Forestry to natural/semi-natural
Natural/semi-natural to natural/semi-natural
Miscanthus to natural/semi-natural
SRC to natural/semi-natural

Arable to miscanthus
Grassland to miscanthus
Forestry to miscanthus
Natural/semi-natural to miscanthus
Miscanthus to miscanthus
SRC to miscanthus

Arable to SRC
Grassland to SRC
Forestry to SRC
Natural/semi-natural to SRC
Miscanthus to SRC
SRC to SRC

Decade 2

Arable to arable
....

Decade 3
 Arable to arable

Decade 4
 Arable to arable

Decade 5
 Arable to arable

Decade 6
 Arable to arable

Decade 7 (LU change projections using decade 6)
 Arable to arable

Carbon change for all soils in the cell (kt C km⁻² 10years⁻¹)
 Decade 1
 Decade 2
 Decade 3
 Decade 4
 Decade 5
 Decade 6
 Decade 7 (LU change projections using decade 6)

Carbon change for organic soils in the cell only (kt C km⁻² 10years⁻¹)
 Decade 1
 Decade 2
 Decade 3
 Decade 4
 Decade 5
 Decade 6
 Decade 7 (LU change projections using decade 6)

D2.3 Format of Output File for C Change data (“CHANGE.OUT”)

For each 20km² grid cell, results are given for the profile to the depth specified in line 9 of G NAMES.DAT

Lines 1: Title line

Lines 2 to end: ID of 20km² grid containing the cell,

Series,

Land use 1

Land use 2

Fraction of first 1km² cell in 20km² grid that changes from LU1 to LU2 in decade 5(??)

For each decade (1-7)

C Change (t C / ha / decade)

CO₂ emission (t C / ha / decade)

CH₄ emission (t C / ha / decade)

N₂O emission (t C / ha / decade)

Total GHG emission in CO₂ equivalents (t C / ha / decade)

Carbon content of soil at start (%C)

Clay content (% clay)

Error in simulation? (0=No; 1=Yes).

D2.4 Format of Climate Change Results file

For each 1km² grid cell, results are given for the profile to the depth specified in line 9 of G NAMES.DAT

Line 1: Title line

Lines 2 to end: ID of 20km² grid containing the cell,
Easting,
Northing,
Carbon change per land use (t C km⁻² 10years⁻¹)
Decade 1
Arable
Grassland
Forestry
Natural/semi-natural
Miscanthus
SRC

Decade 2-7
Arable...

D2.5 Format of File for Calculation of Effects of Different Mitigation Options (files named MIT_A2P.OUT etc)

For each 1km² grid cell, results are given for the profile to the depth specified in line 9 of G NAMES.DAT

Lines 1 and 2: Title lines

Lines 3 to end: ID of 20km² grid containing the cell,
Easting,
Northing,
Dominant soil series 1-5...
Wetness class
% C in top soil layer
% clay in top soil layer
Fraction 1km² cell that has this land use (km²/km²)
Decade 1-7...
Carbon change associated with LU change applied in first decade (t C / ha / km² / decade)

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