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Parsimonious modelling of nutrient fluxes for a terrestrial ecosystem on Svalbard

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Abstract. MBL-MEL, a simple model of ecosystem biogeochemistry, is amended and applied to plant and soil C, ^{14}N and ^{15}N data for the summers of 2001–2003 from Brandalpynten, a maritime high Arctic site on Svalbard following the application of ^{15}N (99 atom%) as $^{15}NO_3$-N at or $^{15}NH_4$-N at concentrations of 1 or 5 kg N ha^{-1}. Variants of this Parent model are also developed to incorporate: temperature dependence into equations describing nutrient fluxes (Temp model); cryptogams (Cryp model); both features combined (CrypTemp model). Goodness-of-fit (GOF) statistics suggest that the addition of temperature-dependence improves the utility of models with and without cryptogams: the residual weighted sums of squares per data point were 5.69, 3.91, 4.31 and 3.93 for the Parent, Temp, Cryp and CrypTemp models respectively. The application of model selection criteria confirm that the addition of temperature-dependence also improves model generalisability. Across all models, the principal discrepancies between observation and prediction are associated with the inorganic soil ^{15}N pool. We conclude that models in which fluxes are described using simple equations that can be augmented to include additional complexity, are an ideal starting point from which the relationship between GOF and model generalisability can be assessed.

Introduction

Research output in the field of modelling terrestrial carbon (C) and nitrogen (N) fluxes favours case-studies in cropland compared to the aggregate semi-natural and natural terrestrial (ASNNT) environment possibly because of missing markets for ecological goods and services (Stapleton et al. 2004). Consequently there is an economic justification for increasing the research output in this field for the ASNNT environment. However there is also a need to ensure that traditional goodness-of-fit (GOF) determinants of model utility are complemented by statistics that can assess whether the complexity of a given model is warranted by the data available. One subset of these statistics are model selection criteria. These criteria penalise the introduction of additional parameters so that a complex model would not be selected over a simpler alternative unless the improvement in fit justifies the extra complexity. Examples include the Akaike information criterion (AIC; Akaike 1973) and the Bayesian information criterion (BIC; Schwarz 1978). Alternative selection criteria are sensitive to the functional form of a model as well as the number of adjustable parameters. Examples of these are the minimum description length (MDL; Rissanen 1987) and the information-theoretic measure of complexity (ICOMP; Bozdogan 1990).

In this paper, a simple model of ecosystem C and N fluxes, MBL-MEL, after Rastetter et al. (1997), is amended and applied to data for five samplings of plant and soil pools taken during the summers of 2001–2003 from ^{15}N (99 atom%) amended plots at Brandalpynten, a maritime high Arctic site on Svalbard. These experiments were carried out to assess the fate and cycling of low but realistic N inputs to the High Arctic. For a comprehensive experimental plan, site description and analysis of data see Tye et al. (2005). The amended MBL-MEL, hereafter the Parent model, is augmented to incorporate temperature-dependence into equations describing fluxes between nutrient pools (Temp model). The Parent model is also extended to include cryptogams in nutrient cycling with and without temperature-dependence, denoted as

Cryp and CrypTemp, respectively. The merit of adding temperature-dependence to both the Parent and Cryp models is judged in terms of both how this improves model GOF and model generalisability as measured using model selection criteria.

Field site, sampling and data

Brandalpynten (78 °56′28″ N; 11 °51′41″ E) is situated on a raised beach terrace dipping to the north and east on the south shore of the Kongsfjorden, near Ny-Ålesund. The area receives an average annual precipitation of 380 mm with the major portion falling between September and April as snow. Annual temperature variation follows a maritime high latitude oscillation with temperatures falling near or below −10 °C in winter. Vegetation at Brandalpynten is composed mainly of subterranean willow (*Salix polaris*), mosses, and saxifrage. The soil profile consists of a humus layer 2–3 cm in depth overlying sandy sub-soil.

The study site was divided into four blocks, each containing five plots (2.5 m × 4.5 m). In each block, one plot received no additional N (control), two plots received $^{15}NH_4$-N at application rates of either 1 kg or 5 kg N ha^{-1}, and two plots received $^{15}NO_3$-N at either 1 kg ha^{-1} or 5 kg ha^{-1} giving a total of four replicate plots for each treatment. The ^{15}N was applied once only, soon after snow melt in 2001 on the 28th and 29th June. The chronology of ecosystem events at Brandalpynten, with their associated model time points based on a monthly timestep, is given in Table 1; the boundaries of the active growing season are 18th June to 17th September in each year (Winther et al. 2002).

A Genstat® 6.1 Repeated Runs ANOVA of the data from Brandalpynten showed that the C and N pools measured in plant and soil fractions in ^{15}N-amended plots were not significantly different from those measured in the control plots ($p > 0.05$). Accordingly the models developed here were tested against data averaged over the control and ^{15}N-amended plots (Table 2). A study examining the response of the microbial community over the same time period, similarly illustrated a lack of response to N amendment (Stapleton et al. 2005).

Table 1. Chronology of ecosystem events at Brandalpynten.

Date	Event	Model t =
18 June 2001	Start 2001 growing season	0
28 June 2001	^{15}N Application	0.327
14–19 July 2001	Sampling 1-2001	0.916
18–21 August 2001	Sampling 2-2001	2.029
18 June 2002	Start 2002 growing season	3
8–12 July 2002	Sampling 1-2002	3.731
9–14 August 2002	Sampling 2-2002	4.778
18 June 2003	Start 2003 growing season	6
9–14 July 2003	Sampling 1-2003	6.774

The 'Model t = 'column illustrates how these different dates translate into model time points based on a monthly time-step where only the active growing season is modelled in each year.

Model descriptions

The Parent model

The Parent model consists of four pools representing organic C and N in humus and vascular plants and a pool representing inorganic soil N. Initial values of these pools are based on the average value across ^{15}N-amended and control plots as determined during Sampling 1 (Model t = 0.916 in Table 2). The transfers between these pools, described by first-order ordinary differential equations, are regulated by ecosystem fluxes of C and N:

Table 2. Plant–soil C (gC m^{-2}), ^{14}N and ^{15}N (gN m^{-2}) pool sizes at Brandalpynten (2001–2003).

Sampling	Model *t*	VegC	SE	VegN	SE	HumusC	SE	HumusN	SE	InorganicN	SE
Jul 01	0.916	61.67	8.990	2.344	3.131E−1	399.6	41.23	26.71	2.671	2.765E−2	6.095E−3
Aug 01	2.029	50.23	5.046	1.736	1.736E−1	*	*	26.76	2.676	1.655E−2	1.655E−3
Jul 02	3.731	42.78	4.526	1.549	1.549E−1	*	*	27.31	2.731	2.892E-2	3.015E−3
Aug 02	4.778	43.57	4.357	1.496	1.496E−1	482.6	48.26	35.28	3.528	3.020E−2	3.020E−3
Jul 03	6.774	38.23	3.858	1.479	1.479E−1	*	*	30.69	3.069	*	*
Sampling	Model *t*	Veg^{15}N-1	SE	Veg^{15}N-5	SE	Humus^{15}N-1	SE	Humus^{15}N-5	SE		
Jul 01	0.916	4.328E−3	5.097E−4	3.541E−2	6.409E−3	1.885E−2	1.885E−3	1.267E−1	1.267E−2		
Aug 01	2.029	4.195E−3	1.070E−3	2.706E−2	6.339E−3	3.965E−2	9.158E−3	8.972E−2	1.391E−2		
Jul 02	3.731	3.172E−3	6.420E−4	3.809E−2	8.619E−3	2.307E−2	2.464E−3	1.400E−1	1.591E−2		
Aug 02	4.778	3.512E−3	5.756E−4	2.234E−2	3.379E−3	2.998E−2	3.377E−3	9.972E−2	9.972E−3		
Jul 03	6.774	3.079E−3	4.225E−4	2.134E−2	4.263E−3	2.507E−2	2.507E−3	1.006E−1	1.006E−2		
Sampling	Model *t*	Inorganic^{15}N-1	SE	Inorganic^{15}N-5	SE	CrypC[a]	SE[a]	CrypN[†]	SE[a]		
Jul 01	0.916	1.224E−4	1.882E−5	1.353E−3	3.118E−4	350.5	35.05	10.24	1.024		
Aug 01	2.029	1.643E−4	3.565E−5	5.761E−4	7.564E−5	462.1	46.21	13.72	1.372		
Jul 02	3.731	8.254E−5	8.254E−6	5.425E−4	6.837E−5	359.0	35.90	10.26	1.248		
Aug 02	4.778	9.052E−5	1.789E−5	3.698E−4	8.695E−5	391.1	59.51	11.34	1.272		
Jul 03	6.774	*	*	*	*	331.5	33.15	9.96	0.996		
Sampling	Model *t*	Cryp^{15}N-1	SE	Cryp^{15}N-5	SE						
Jul 01	0.916	3.100E−2	3.670E−3	1.343E−1	1.763E−2						
Aug 01	2.029	3.607E−2	4.941E−3	1.550E−1	3.539E−2						
Jul 02	3.731	2.255E−2	4.447E−3	1.204E−1	1.780E−2						
Aug 02	4.778	3.490E−2	8.190E−3	1.115E−1	2.306E−2						
Jul 03	6.774	3.405E−2	4.172E−3	1.357E−1	1.646E−2						

C and ^{14}N data are averages across control and ^{15}N-amended plots. [a]Denotes Cryp and CrypTemp models only.

$$\frac{\mathrm{dVegC}}{\mathrm{d}t} = \mathrm{UptakeC} - \mathrm{LitterC} - \mathrm{VegResp}$$

$$\frac{\mathrm{dVegN}}{\mathrm{d}t} = \mathrm{UptakeN} - \mathrm{LitterN} - \mathrm{ReleaseN}$$

$$\frac{\mathrm{dHumusC}}{\mathrm{d}t} = \mathrm{LitterC} - \mathrm{MicroResp}$$

$$\frac{\mathrm{dHumusN}}{\mathrm{d}t} = \mathrm{LitterN} + \mathrm{ImmobN} - \mathrm{MinN}$$

$$\frac{\mathrm{dInorganicN}}{\mathrm{d}t} = \mathrm{InputN} + \mathrm{MinN} + \mathrm{ReleaseN} - \mathrm{LeachingN} - \mathrm{ImmobN} - \mathrm{UptakeN}$$

where UptakeC, UptakeN = uptake of inorganic C [N] by vegetation (gC[N] $m^{-2}mo^{-1}$), LitterC, LitterN = litter loss of organic C [N] from vegetation (gC[N] m^{-2} mo^{-1}), VegResp, MicroResp = vegetation and microbial respiration (gC m^{-2} mo^{-1}), ReleaseN = inorganic release of N from vegetation (gN m^{-2} mo^{-1}), MinN, ImmobN = gross mineralisation and immobilisation of N (gN m^{-2} mo^{-1}), InputN, LeachingN = inorganic replenishment and leaching loss of N (gN m^{-2} mo^{-1}).

Of these 11 fluxes, 8 are described by first-order kinetics. The initial values of rate-coefficients for these first-order processes are back-calculated so that the system is at a steady-state prior to the application of ^{15}N. Steady-state in the MBL-MEL is calculated based on certain assumptions of relative nutrient flow (Table 3) that are applied to the Parent model.

Steady-state in the C component of the Parent model is based on a determination of MicroResp from which the size of the remaining C fluxes is calculated using the proportionality factors in Table 3. Nakatsubo et al. (1998) report microbial respiration rates for various sites around Ny Ålesund from which an average respiration rate for Brandalpynten was calculated as 8.335 gC m^{-2} mo^{-1}. Therefore to remain at a steady-state UptakeC, VegResp and LitterC need to equal 16.67, 8.335 and 8.335 gC m^{-2} mo^{-1} respectively in the Parent model.

Steady-state in the N component of the Parent model is based on a determination of UptakeN. Shaver and Chapin (1991) report plant uptake of N in a cognate ecosystem as 0.56 gN m^{-2} mo^{-1}. Therefore to remain at a steady-state ReleaseN, LitterN, MicroUptakeN and MinN need to equal 0.112, 0.448, 0.448 and 0.896 g Nm^{-2} mo^{-1} respectively in the Parent model.

The values of InputN and LeachingN are calculated independently, which preserves the steady-state provided they are equal in magnitude. There is little time-series data on N deposition on Svalbard. Joranger and Semb (1989) report N deposition at Ny Ålesund as 0.05 gN m^{-2} between August 1982 and July 1983 and 0.15 gN m^{-2} between August 1983 and July 1984. This latter figure is still widely used to express contemporary N deposition despite being dated (e.g. Woodin 1997; Gordon et al. 2001). In 2001 snowpack N at Brandalpynten was measured as 0.009 gN m^{-2}. Considering that the majority of annual aerial deposition will accumulate in the snowpack over the long winter this figure is surprisingly low compared to

Table 3. Relative nutrient fluxes in MBL-MEL as derived by Rastetter et al. (1997).

C flux		N flux	
UptakeC	1	UptakeN	1
VegResp	0.5	ReleaseN	0.2
MicroResp	0.5	LitterN	0.8
LitterC	0.5	MinN	1.6
		ImmobN	0.8

data reported by Joranger and Semb (1989) and calls into question the assumption that snowmelt provides a significant pulse of nutrients to high Arctic ecosystems. It is assumed in the Parent model that 0.009 gN m^{-2} is deposited every month over the 3 month growing season i.e. initial nutrient pulse = subsequent monthly summer deposition rate. This may appear to overestimate summer deposition based on the snowpack data. However it would be difficult to justify using a lower figure. Therefore at steady-state, InputN = LeachingN = 0.009 gN m^{-2} mo^{-1}.

Steady-state values for rate-coefficients in the Parent model are given in Table 4. InputN, UptakeC and UptakeN are processes that are not defined by first-order kinetics. InputN, as discussed, is a defined magnitude and therefore omitted from Table 4. UptakeC and UptakeN are Michaelis–Menten functions of element concentration:

$$\mathrm{UptakeC} = \frac{\mathrm{gC} \times \mathrm{UpEffortC} \times \mathrm{CO_2}}{k\mathrm{C} + \mathrm{CO_2}}$$

$$\mathrm{UptakeN} = \frac{\mathrm{gN} \times \mathrm{UpEffortN} \times \mathrm{InorganicN}}{k\mathrm{N} + \mathrm{InorganicN}}$$

where UpEffortC, UpEffortN = an acclimation mechanism (unitless), gC, gN = plant uptake parameter for C [N] (gC[N] m^{-2} mo^{-1}), kC, kN = half saturation constant for C [N] (gC[N] m^{-2}), CO_2 is the atmospheric concentration of carbon (gC m^{-3}). This value is based on Mauna Loa CO_2 data for 2001 (Keeling and Whorf 2005).

The acclimation mechanism ensures that transfer of C and N to the plant depends on the substrate and plant concentrations of both nutrients. It constrains the vegetation within a nutritional balance by regulating the C–N ratio through changes in the uptake effort applied to either nutrient (Rastetter et al. 1997). Mathematically, changes in uptake effort applied to C and N acquisition are represented as:

$$\frac{\mathrm{dUpEffortC}}{\mathrm{d}t} = -a \times A \times \mathrm{UpEffort}^*$$

$$\mathrm{UpEffort}^* = \mathrm{UpEffortC} \quad \text{if} : A > 0$$

$$\mathrm{UpEffort}^* = \mathrm{UpEffortN} \quad \text{if} : A < 0$$

$$\frac{\mathrm{dUpEffortN}}{\mathrm{d}t} = -\frac{\mathrm{dUpEffortC}}{\mathrm{d}t}$$

where

$$A = \ln \frac{\mathrm{VegC}}{\varepsilon \times \mathrm{VegN}} + \tau(\mathrm{GrC} - \mathrm{GrN})$$

$$\mathrm{GrC} = \frac{\mathrm{dVegC}}{\mathrm{d}t} \times \frac{1}{\mathrm{VegC}}$$

$$\mathrm{GrN} = \frac{\mathrm{dVegN}}{\mathrm{d}t} \times \frac{1}{\mathrm{VegN}}$$

Table 4. Steady-state values of rate-coefficients in the Parent, Temp, Cryp and CrypTemp models.

Model	Process	Parameter	Value	Units
Parent	UptakeC	gC	76.03	gC m^{-2} mo^{-1}
	UptakeN	gN	5.819	gN m^{-2} mo^{-1}
	VegResp	rC	1.352E−1	gC m^{-2} mo^{-1}
	ReleaseN	rN	4.778E−2	gN m^{-2} mo^{-1}
	MicroResp	rC2	2.086E−2	gC m^{-2} mo^{-1}
	LitterC	mC	1.352E−1	gC m^{-2} mo^{-1}
	LitterN	mN	1.911E−1	gN m^{-2} mo^{-1}
	MinN	rN2	3.354E−2	gN m^{-2} mo^{-1}
	ImmobN	gN2	16.20	gN m^{-2} mo^{-1}
	LeachingN	βNe	3.255E−1	gN m^{-2} mo^{-1}
Temp	UptakeC	gC	215.9	gC m^{-2} mo^{-1}
	UptakeN	gN	16.52	gN m^{-2} mo^{-1}
	VegResp	rC	8.801E−1	gC m^{-2} mo^{-1}
	ReleaseN	rN	1.357E−1	gN m^{-2} mo^{-1}
	MicroResp	rC2	7.533E−2	gC m^{-2} mo^{-1}
	LitterC	mC	1.352E−1	gC m^{-2} mo^{-1}
	LitterN	mN	1.911E−1	gN m^{-2} mo^{-1}
	MinN	gN2	58.50	gN m^{-2} mo^{-1}
	ImmobN	rN2	1.211E−1	gN m^{-2} mo^{-1}
	LeachingN	βNe	3.255E−1	gN m^{-2} mo^{-1}
Cryp	CrypUptakeC	gC2	38.01	gC m^{-2} mo^{-1}
	CrypResp	rC3	2.378E−2	gC m^{-2} mo^{-1}
	CrypReleaseN	rN3	5.078E−5	gN m^{-2} mo^{-1}
	CrypLitterC	mC2	2.378E−2	gC m^{-2} mo^{-1}
	CrypLitterN	mN2	2.031E−4	gN m^{-2} mo^{-1}
	UptakeC	gC	76.03	gC m^{-2} mo^{-1}
	UptakeN	gN	5.819	gN m^{-2} mo^{-1}
	VegResp	rC	1.352E−1	gC m^{-2} mo^{-1}
	ReleaseN	rN	4.778E−2	gN m^{-2} mo^{-1}
	MicroResp	rC2	4.172E−2	gC m^{-2} mo^{-1}
	LitterC	mC	1.352E−1	gC m^{-2} mo^{-1}
	LitterN	mN	1.911E−1	gN m^{-2} mo^{-1}
	MinN	rN2	3.369E−2	gN m^{-2} mo^{-1}
	ImmobN	gN2	16.28	gN m^{-2} mo^{-1}
	LeachingN	βNe	3.255E−1	gN m^{-2} mo^{-1}
CrypTemp	CrypUptakeC	gC2	446.4	gC m^{-2} mo^{-1}
	CrypResp	rC3	2.793E−1	gC m^{-2} mo^{-1}
	CrypReleaseN	rN3	5.96E−4	gN m^{-2} mo^{-1}
	CrypLitterC	mC2	1.506E−2	gC m^{-2} mo^{-1}
	CrypLitterN	mN2	58.79	gN m^{-2} mo^{-1}
	UptakeC	gC	215.9	gC m^{-2} mo^{-1}
	UptakeN	gN	16.52	gN m^{-2} mo^{-1}
	VegResp	rC	8.801E−1	gC m^{-2} mo^{-1}
	ReleaseN	rN	1.357E−1	gN m^{-2} mo^{-1}
	MicroResp	rC2	1.217E−1	gN m^{-2} mo^{-1}
	LitterC	mC	1.352E−1	gC m^{-2} mo^{-1}
	LitterN	mN	1.911E−1	gN m^{-2} mo^{-1}
	MinN	rN2	446.4	gC m^{-2} mo^{-1}
	ImmobN	gN2	2.793E−1	gC m^{-2} mo^{-1}
	LeachingN	βNe	3.255E−1	gN m^{-2} mo^{-1}

All parameters are adjustable under model fitting.

$$\varepsilon = \frac{\varepsilon\text{stems} \times \text{VegC}}{k\varepsilon + \text{VegC}}$$

A description of the variables, parameters and values used in the definition of UptakeC and UptakeN is provided in Table 5. The values given are self-explanatory with two exceptions: the allometric parameter ($k\varepsilon$) is set so that the optimum C–N ratio (ε) equals the initial C–N ratio (ε = VegC/VegN) at the initial value of VegC (Rastetter et al. 1997).

The mechanics outlined here differ somewhat from the original MBL-MEL. First, terms for the vegetation surface that is active in the uptake of C and N (SC, SN) from the numerators of UptakeC and UptakeN, have been removed. These variables required morphological constants for C and N that are difficult to quantify accurately for ecosystems where there is no single dominant species, hence their exclusion from the Parent model UptakeC and UptakeN functions.

Secondly, MBL-MEL represented microbial respiration and mineralisation/immobilisation dynamics in a relatively complex manner, which was unstable when applied to our dataset: the required mineralisation/immobilisation dynamics could only be reproduced by using unrealistic parameter values. Hence the reformulation of MicroResp, MinN, ImmobN to first-order relationships as discussed above. This approach to the modelling of soil nutrient dynamics could result in unrealistic deviations from the optimal C–N ratio if the model were used to make predictions beyond the period covered by our available data. However, as a first-approximation it is advantageous because of its inherent simplicity.

^{15}N dynamics are based upon those of ^{14}N. The ^{15}N pools are initially set to zero and transfers between them assume that the ^{15}N behaves as ^{14}N and therefore fluxes are in the same proportion. For example,

$$\text{Uptake}^{15}\text{N} = \left(\frac{\text{UptakeN}}{\text{InorganicN}}\right) \times \text{Inorganic}^{15}\text{N}$$

The Temp model

Physiological processes regulating the size of C and N pools are temperature sensitive and temperature response functions (TRFs) can be incorporated into the mathematical descriptions of these processes to increase the mechanistic credibility of the Parent model. The TRFs used here are derived from Lassiter (1975) and used subsequently in MBL-GEM (Rastetter et al. 1991). They take the following functional form:

Table 5. Steady-state UptakeC and UptakeN parameterisation for the Parent, Temp, Cryp and CrypTemp models.

Variable[a]/ Parameter	Description	Value	Unit	Source
A[a]	Acclimation potential	0	Unitless	Rastetter et al. (1997)
a	Acclimation rate	4.167E−1	mo^{-1}	Rastetter et al. (1997)
GrC[a]	Relative C growth rate	0	mo^{-1}	Calculated
GrN[a]	Relative N growth rate	0	mo^{-1}	Calculated
kC	Half saturation constant for C	475	gC m^{-2}	McKane et al. (1997)
kN	Half saturation constant for N	1.16E−1	gN m^{-2}	McKane et al. (1997)
$k\ \varepsilon$	Allometric parameter	204.6	g m^{-2}	Back-calculated
ε[a]	Optimal element ratio	26.31	g^{g-1}	Calculated
εstems	Element ratio of stems	113	g^{g-1}	McKane et al. (1997)
UpEffortC[a]	Uptake effort allocated to C by vegetation	5E−1	Unitless	Rastetter et al. (1997)
UpEffortN[a]	Uptake effort allocated to N by vegetation	5E−1	Unitless	Rastetter et al. (1997)
τ	Acclimation damping coefficient	25E−1	mo^{-1}	Rastetter et al. (1997)

Uptake parameters for C and N (gC, gN) are different between models to preserve the steady-state (see Table 4).

$$QX(T) = e^{qX(T-T_{OX})}\left(\frac{T_{MX}-T}{T_{MX}T_{OX}}\right)^{qX(T_X-T_{OX})}$$

where qX = curvature parameter (°C^{-1}), T = temperature (°C), T_{MX} = maximum temperature (°C), T_{OX} = optimum temperature (°C).

For

$$X = \text{UptakeC, MicroResp, UptakeN, ReleaseN, MinN, ImmobN}$$

For UptakeC, UptakeN, VegResp and MicroResp the same maxima and optima estimates used in McKane et al. (1997) have been used (supplied by RB McKane, pers. commun.). However, the values of the curvature parameters (q) have been amended as the originals used by McKane et al. (1997) significantly overestimate the relative rate of physiological processes at 0 °C when compared to the graphical representations of these functions given in that work. Alteration of these parameters (Table 6) was accomplished using the Solver function in Microsoft Excel® 9.0, resulting in very similar function curvature to an alternative procedure adopted by McKane et al. (1997), which involved introducing an intercept correction parameter.

There is a lack of data pertaining to the temperature response of N release from plant roots. Accordingly, we assumed that the temperature response of ReleaseN was the same as that for UptakeC and UptakeN. Marion and Black (1987) and Schmidt et al. (1999) report highly variable estimates in terms of the temperature response of mineralisation and immobilisation respectively. Accordingly the TRF for microbial respiration has been generalised to these two processes. This approach is supported by Thamdrup and Fleischer (1998) who report a similar temperature dependency across mineralisation and microbial respiration in Svalbard aquatic sediments.

Ambient daily air temperature for 2001–2003 growing seasons (Norwegian Meteorological Institute, pers. commun.) is used as input data for the TRFs associated with UptakeC, UptakeN, VegResp and ReleaseN. Data loggers provided daily temperature data for the humus layer during the 2002 growing season. Given that humus temperature correlates closely with ambient air temperature, humus temperature data for the 2001 and 2003 growing seasons were extrapolated from ambient air temperature data with a +0.4 °C correction factor; this is used as input data for the TRFs associated with MicroResp, MinN and ImmobN. Over 2001–2003 growing seasons, air temperature (humus temperature) ranged between a minimum of −4.4 °C (−4.8 °C) on 7th September 2002 and a maximum of 10.9 °C (11.3 °C) on 9th August 2001.

Finally, incorporating temperature-dependence into physiological processes requires adjustment of the rate-coefficients in these processes at initialisation in order for the system to remain at a steady-state prior to model fitting (Table 4).

The Cryp model

Extending the Parent model to incorporate cryptogams required adding two pools to represent C and N in cryptogam biomass: CrypC and CrypN. The initial value of these pools is based on the average value across N-amended and control plots as determined during Sampling 1 (Table 2).

Table 6. Temperature response parameters utilised in McKane et al. (1997) including original and amended curvature parameter (q) estimates.

	Optimum (°C)	Maximum (°C)	Old q (°C^{-1})	New q (°C^{-1})
UptakeC	20	40	9.669E−2	2.622E−1
UptakeN	20	40	9.669E−2	2.622E−1
VegResp	35	50	8.71E−2	1.359E−1
MicroResp	24	50	1.022E−1	2.711E−1

Photosynthesis is similar across cryptogams and most polar vascular plants (Lloyd 2001) but these plant types have distinct ways of accessing N: cryptogams derive N from aerial deposition as opposed to uptake from soil. In the model, cryptogamic photosynthesis is defined as:

$$\mathrm{CrypUptakeC} = \frac{\mathrm{gC2} \times \mathrm{CO_2}}{k\mathrm{C2} + \mathrm{CO_2}}$$

where gC2 = cryptogam uptake parameter for C (gC m^{-2} mo^{-1}), kC2 = half saturation constant for C (gC m^{-2}). kC2 is set as 475 gC m^{-2} as per vascular plants in Table 5. UpEffortC, which appears in the numerator of the UptakeC function, has been excluded here because an acclimation mechanism based on N is not appropriate to cryptogams given their passive aerial absorption of N. As was the case with our representation of soil nutrient dynamics, this could result in unrealistic deviations from the optimal C–N ratio if model predictions are extrapolated beyond the period covered by our time-series data. Cryptogamic respiration and C loss in litterfall are defined as first-order processes in the same manner as vascular plants. The steady-state magnitudes of these three cryptogamic C fluxes are set equal to the vascular plant equivalents, enabling back-calculation of these rate-coefficients at steady-state (Table 4). Addition of cryptogams doubles the C input into the HumusC pool (i.e. CrypLitterC). Therefore to remain at steady-state, the size of the rate-coefficient associated with MicroResp has to double from the Parent model magnitude (Table 4).

Uptake of N by cryptogams is defined as:

$$\mathrm{CrypUptakeN} = 0.289 \times \mathrm{InputN}$$

This is based upon the average proportion of the applied ^{15}N recovered in cryptogams at Sampling 1. Therefore in terms of aerial ^{14}N deposition, 0.0026 gN m^{-2} mo^{-1} of the 0.009 gN m^{-2} mo^{-1} is determined to be deposited on cryptogams. Loss of N from cryptogams is dependent upon two first-order rate processes: CrypReleaseN and CrypLitterN. At steady-state the magnitudes of these coefficients (Table 4) are based on the same proportions as in the Parent model where 80% of N is lost through LitterN and 20% lost through ReleaseN. The N lost in cryptogamic litter represents an additional input into the HumusN pool: total input into this pool is therefore 0.45 gN m^{-2} mo^{-1} compared to 0.448 gN m^{-2} mo^{-1} in the Parent model. This requires MinN = 0.9 gN m^{-2} mo^{-1} and ImmobN = 0.45 gN m^{-2} mo^{-1} at steady-state (Table 4). This is an increase in net mineralisation of 0.002 gN m^{-2} mo^{-1} compared to the Parent model. CrypReleaseN is also adding 0.00052 gN m^{-2} mo^{-1} to the InorganicN pool. The sum of these two magnitudes together with the 0.0064 gN m^{-2} mo^{-1} of aerially deposited N received directly by the soil in this model formulation totals 0.009 gN m^{-2} mo^{-1}, which is steady-stated with LeachingN.

The CrypTemp model

The inclusion of both cryptogams and temperature-dependence requires the further addition of temperature-dependence to three processes: CrypResp; CrypUptakeC; CrypReleaseN. These TRFs are of the same functional form as used in the Temp model. The same optima, maxima and curvature parameters have been applied across all three processes: optima 18 °C; maxima 35 °C; q 0.7 $°C^{-1}$. This is based on various sources (e.g. Skre and Oechel 1981; Harley et al. 1989; Lange et al. 1996) with manipulation of the q value as per the Temp model.

In CrypTemp, rate-coefficients associated with those Parent model processes incorporating a TRF remain unchanged from the Temp model excepting MicroResp, MinN and ImmobN where the addition of cryptogams altered the size of these fluxes at steady-state (Table 4).

Model implementation and fitting

The models differential equations were solved using the 4th order Runge–Kutta procedure (Press et al. 2002) over a 3 year simulation (nine growing season months). Initial values and external drivers were as defined in the model description sections above.

Certain poorly defined parameters were fitted using the Marquardt method (Press et al. 2002) in order to minimise the deviation between prediction and observation. This is limited to all of the rate-coefficients in Table 4 that were back-calculated at model initialisation to permit a steady-state where inputs of C and N = outputs of C and N. The common adjustable parameters across all model variants are: the leaching loss parameter (βNe); the plant uptake parameters for C and N (gC and gN); N immobilisation and mineralisation parameters (gN2 and rN2); plant litter loss parameters (mC and mN); vegetation and microbial respiration parameters (rC and rC2); a vegetation inorganic N release parameter (rN). The addition of cryptogams in the Cryp and CrypTemp models presents five additional adjustable parameters: the cryptogam uptake parameter for C (gC2); cryptogam litter loss parameters (mC2 and mN2); cryptogam respiration and inorganic N release parameters (rC3 and rN3).

Fitting constraints for most adjustable parameters were set at $\pm$factor 5 of their steady state value. Exceptions are those adjustable parameters associated with cryptogamic C fluxes: gC2, mC2 and rC3. In these cases the fitting constraints are $-$factor 5, $+$factor 10 of their steady state values. This is to account for the fact the CrypC pool is significantly bigger than the VegC pool; the initial steady state, where C fluxes are the same magnitude for both plant types, may underestimate cryptogamic C fluxes more than vascular plants.

This type of parameter search is open to the risk of identifying local, rather than global minima in the residual sum of squares surface. Therefore the resulting parameter values were checked against those obtained using a simulated annealing search procedure to give confidence that we had located the global minimum in each case.

Certain parameters common across all model variants are fixed (Table 5): the acclimation rate parameter and acclimation damping coefficient (a and τ); the half saturation constants for plant uptake of C and N (kC and kN); element ratio of stems qstems); the allometric parameter (kq). The half saturation constant for cryptogam uptake of C (kC2) is fixed in Cryp and CrypTemp.

There are no new adjustable parameters associated with the addition of temperature-dependence in the Temp and CrypTemp models compared to the Parent and Cryp models respectively. Although some of the TRFs are estimated with a high degree of uncertainty, allowing parameters within these TRFs to be adjustable under model fitting would produce significant redundancy as those processes that incorporate a TRF in the Temp and CrypTemp models already contain one adjustable parameter as per the Parent and Cryp models, respectively.

Results

Goodness-of-fit

The residual weighted sums of squares (RWSS) per data point are 5.69, 3.91, 4.31 and 3.93 for the Parent, Temp, Cryp and CrypTemp models respectively (Table 7). This is calculated across all state variables with weights taken as the reciprocal of measurement errors. Therefore, the addition of temperature-dependence into physiological processes improves the fit of the Parent and Cryp models with Temp and CrypTemp resulting in RWSS per data point values that were 69 and 91% of the values recorded for the Parent and Cryp model respectively. Across all models, the principal discrepancies between observation and prediction are associated with the Inorganic^{15}N pools (Figures 1 and 2) where all models predict lower concentrations than observed at the various samplings.

Parameters: standard errors and correlations

Most fitted parameters showed limited variability across the Parent model and variants. However, standard errors (SEs) are generally high for the parameter estimates across all four models, which undermines their reliability. This is at least in part due to high covariances between many of these fitted parameters. There is one parameter–parameter correlation that is consistently high across all four models: mC–rC in LitterC

Table 7. Goodness of fit (RWSS per data point) for the four models of ecosystem nutrient flux.

Model	Data points	Adjustable parameters	Degrees of freedom	RWSS/Data points
Parent	49	10	39	5.69
Temp	49	10	39	3.91
Cryp	69	15	54	4.31
CrypTemp	69	15	54	3.93

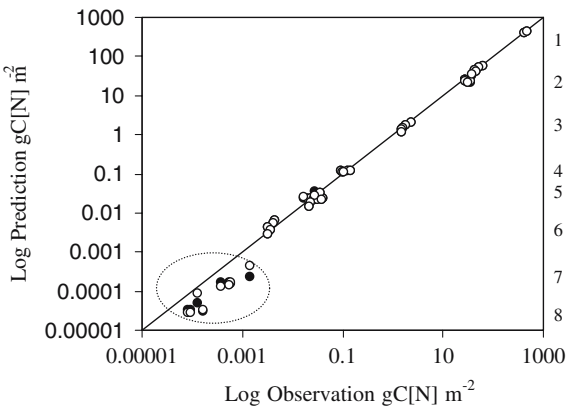

Figure 1. Log prediction – log observation in the Parent (○) and Temp (●) models. The solid diagonal is a 1-1 line where observation and prediction are equal. Eight clusters based on magnitude are identified: (1) HumusC; (2) VegC, HumusN; (3) VegN; (4) Humus^{15}N-5; (5) InorganicN, Veg^{15}N-5, Humus^{15}N-1; (6) Veg^{15}N-1; (7) Inorganic^{15}N-5; (8) Inorganic^{15}N-1. The ellipse highlights the Inorganic^{15}N clusters where the discrepancy between observation and prediction is highest.

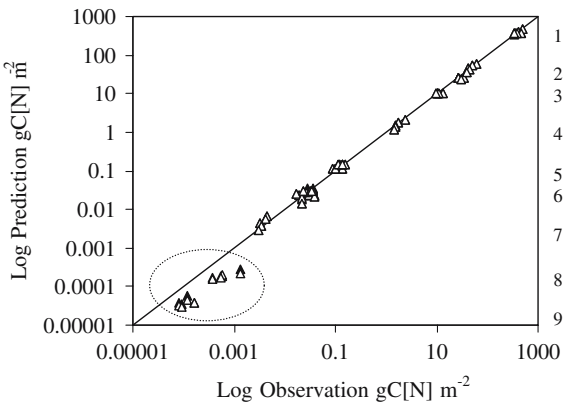

Figure 2. Log prediction – log observation in the Cryp (△) and CrypTemp (▲) models. The solid diagonal is a 1–1 line where observation and prediction are equal. Nine clusters based on magnitude are identified: (1) CrypC, HumusC; (2) VegC, HumusN; (3) CrypN; (4) VegN; (5) Cryp^{15}N-5, Humus^{15}N-5; (6) InorganicN, Veg^{15}N-5, Cryp^{15}N-1, Humus^{15}N-1; (7) Veg^{15}N-1; (8) Inorganic^{15}N-5; (9) Inorganic^{15}N-1. The ellipse highlights the Inorganic^{15}N clusters where the discrepancy between observation and prediction is highest.

and VegResp respectively. The addition of cryptogams in the Cryp and CrypTemp models introduces five adjustable parameters that are not seen in either the Parent or Temp models. Of these cryptogam specific parameters there are two parameter–parameter correlations that are high in both Cryp and CrypTemp: gC2–rC3 in CrypUptakeC and CrypResp; mC2 and rC2 in CrypLitterC and MicroResp.

Table 8. Generalisability statistics applied to the four models of ecosystem nutrient flux.

Model	AIC	BIC	MDL	ICOMP
Parent	708.1	727.0	362.6	397.2
Temp	583.2	602.1	289.0	337.2
Cryp	794.4	827.9	399.5	520.0
CrypTemp	763.7	797.2	376.5	508.8

Model selection

The Parent model is distinct from the Cryp model in terms of the number of data points and the number of adjustable parameters. Therefore, model selection criteria can only be used to compare the Parent with the Temp model and the Cryp with the CrypTemp model. The model that minimises the value of a given statistic should be chosen. The AIC and BIC are included here for heuristic purposes only: these statistics are only sensitive to changes in the number of adjustable parameters, which are constant between Parent and Temp, Cryp and CrypTemp. Temp and CrypTemp yield lower values than the Parent and Cryp models across all four statistics (Table 8). This confirms that the improvements in GOF noted above do not compromise model generalisability.

Discussion

If we accept that GOF is an inadequate sole determinant of model utility then simple models like MBL-MEL appear to be an ideal starting point from which complexity can be systematically added and assessed using model selection criteria. Here, the addition of temperature-dependence into models of ecosystem C and N flux, with and without cryptogams, was a win–win in terms of improving GOF and generalisability. In this respect, the models could be described as parsimonious.

The models as parameterised here represent a compromise between avoiding the risk of over-fitting (given the limitations of the data) and mechanistic credibility. They should be used cautiously but do provide a means to gain insight into the biogeochemistry of the ecosystem under study. A striking feature of this ecosystem was its capacity to capture and retain applied N. For example, c. 60% of the applied N was found in the various plant–soil fractions at less than 3 weeks after the N application, illustrating a rapid conversion to organic forms of N. There is little subsequent change in applied N (i.e. tracer N) over a 3 year period, which indicates highly conservative retention by this ecosystem. In terms of cycling, after the initial partitioning of N there were no significant changes in concentration observed in the plant fractions. However, transfer from the microbial biomass to humus is apparent over time (Tye et al. 2005).

There is scope for investigating the effect of additional features on model performance, such as light intensity and soil moisture that are not currently incorporated in the model variants presented here. Differentiating between humus and microbial biomass pools would also capture the transfer from the former to the latter, stable form of N. If these features can be added without increasing the number of adjustable parameters as was the case with the addition of temperature-dependence, any improvement in GOF is less likely to negatively affect model generalisability through overfitting. The incorporation of such features could also reduce the SE associated with various adjustable parameters in the models developed here, which are currently high.

The alternative modelling approach that dominates in the literature, whereby a highly mechanistic model is applied to a dataset and assessed in terms of GOF, gives no indication as to whether simpler alternatives would have similar GOF and perhaps generalise better.

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