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The ICBM family of analytically solved models of soil carbon, nitrogen and microbial biomass dynamics — descriptions and application examples

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Abstract

Based on the Introductory Carbon Balance Model, ICBM, we present a set of analytically solved models. The original ICBM comprises 'Young' and 'Old' soil C, two decay constants and parameters for litter input,'humification' and external influences — in all five parameters. The new models describe soil C (and N) balances more in detail, but they are built around the same core concepts such as first-order decomposition kinetics and a minimum number of soil C and N pools. More complex processes, such as plant growth and mortality as well as weather influence are not explicitly included. However, these processes are allowed to influence the model predictions by modifying model parameter values. These modifications may be based on 'best guesses', parameter optimisations to available data, or independent 'front-end models', e.g. calculations of temperature influence on decomposer activity. Listed according to increasing complexity, the models are: (1) ICBM/N, which is ICBM with nitrogen added. It calculates net N-mineralisation and adds parameters for C/N ratios and soil organisms as well as organism efficieny — nine parameters in all; (2) ICBM/2N, which gives a more precise description of the initial stages of decomposition by splitting the 'Young' pool into two. The nitrogen part of the model has parameters for the C/N ratios of 'labile' and 'refractory' input of organic material, organism biomass and humification and also microbial growth efficiency for 'labile' and 'refractory'. The model has 13 parameters in all, but can be run as a pure C model (ICBM/2) with only seven parameters; (3) ICBM/2BN, where organism biomass C and N is explicitly modelled. This model is usually run with daily, weekly or monthly steps and adds parameters related to biomass — 18 parameters in total — and can be run as a pure C model (ICBM/2B) with 13 parameters or even as a model with only one 'Young' pool (ICBM/B). We give examples of model applications, both short- and long-term, and show that the models relatively easily can be applied to various, more or less incomplete, data sets. The models do not require simulation techniques and are easily programmed in, e.g. electronic spreadsheets such as Microsoft Excel. By transformation of the time steps even dynamic driving variables, e.g. weather-related, can be applied without simulation. Model equations and ready-to-run programs (Excel, SAS) can be found at http://www.mv.slu.se/vaxtnaring/olle/ICBM.html.

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1. Introduction

Carbon and nitrogen dynamics in the soil can be described by a number of approaches, usually involving simulation modelling (see e.g. Ågren et al., 1991; Chertov and Komarov, 1996; Powlson et al., 1996; Paustian et al., 1997; Fu et al., 2000). The analytical approach to soil carbon modelling, as opposed to simulation, is not new (Hénin and Dupuis, 1945; Hénin et al., 1959; Ågren and Bosatta, 1996), but recent interest in regional and global modelling (often GIS based) has spawned a number of efforts to use simple, analytically solved models.

Andrén and Kätterer (1997) presented the Introductory Carbon Balance Model (ICBM), originally designed to calculate soil carbon balances in a 30-year time perspective. The differential equations were solved analytically, and thus, parameter values could be estimated by using generally available non-linear regression routines, model properties could be mathematically derived, and the model could be used as well as optimised interactively in computer spreadsheet programs.

The objective of the work presented here was to expand the ICBM concept of analytically solved models to also include nitrogen and soil organism biomass dynamics. We give examples of how the ICBM family of models (Fig. 1) can be used to describe, analyse and predict C, N and organism biomass dynamics during short-, medium- and long-term decomposition of organic materials such as litter and older soil organic matter — including a constant input from plant production. We also show how driving variables such as daily temperature and soil moisture under certain assumptions can be used without simulation techniques, by transforming time into 'optimum temperature and moisture time' using any temperature and moisture response function. (See http://www.mv.slu.se/vaxtnaring/olle/ICBM.html for programs in Excel and SAS.)

For a number of reasons, the models are developed with simplicity as the main objective. In contrast to complex simulation models, analyti-

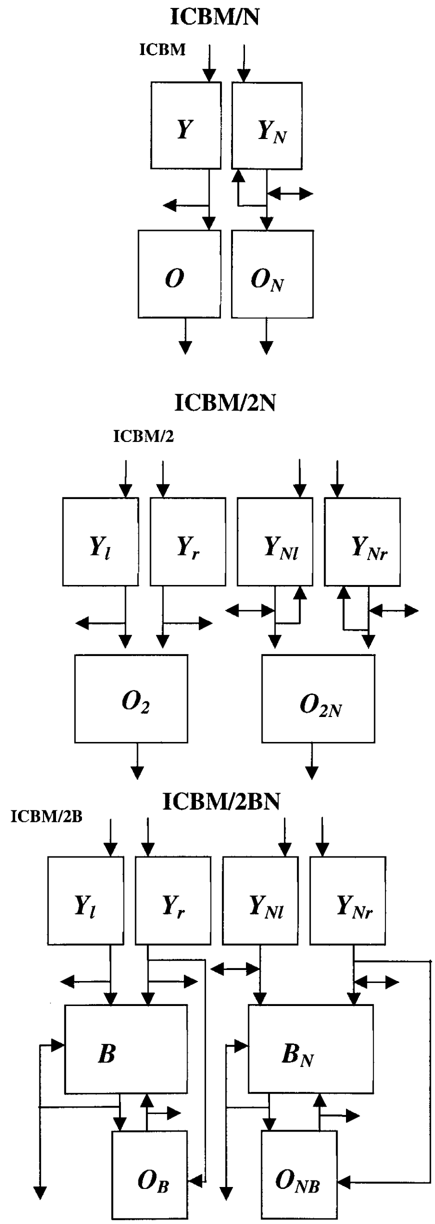

Fig. 1. The ICBM family of models. Arrows not pointing at pools indicate CO_2 emission and nitrogen mineralisation. Double-headed arrows indicate nitrogen mineralisation/immobilisation. (*Y*, 'Young' carbon; *O*, 'Old' carbon; *B*, soil organism biomass carbon. Subscripts: *l*, labile fraction; *r*, refractory fraction; N, organic nitrogen pool).

cally solved models can easily be surveyed and distributed and their outcome can be calculated using a pocket calculator. Less effort is needed to obtain estimates for parameter values. A simple model can also fairly easily be parameterised for large and incomplete data sets (Kätterer and Andrén, 1999), or be run with many parameter settings simultaneously, e.g. in a GIS grid (Andrén, In press), on an ordinary personal computer yielding almost instantaneous outputs.

The disadvantage of a simple model is that so much falls outside the model. We think that this in many cases can be turned into an advantage, since a step-by-step approach to a complex problem often can be the best one. For example, to estimate the annual amount and quality of carbon input to the soil is very hard — no simple, general methods exist. However, if we make our best estimates in this respect, we can easily use these as input to the simple and straightforward soil carbon model and see how they work. Alternatively, we can use the soil carbon model to calculate a probable input — in a sense modelling the unmeasurable (cf. Elliott et al., 1996; Magid et al., 1997).

In the first part of this paper, the ICBM family of models are presented. In the second part, examples are provided, showing how to use these models for analysing soil C and N dynamics at different time scales. A list of all symbols used in the model equations are given in Appendix A and exact analytical solutions to the model equations are provided in Appendix B.

2. Model descriptions

2.1. ICBM

ICBM has two carbon pools (Figs. 1 and 2, 'ICBM'), a 'Young' (Y) and an 'Old' (O). Input to Y (from litter-fall and root death) is usually calculated as fraction of plant production. Outflows from the pools follow first-order kinetics (k_Y, k_O). External (climate, soil type, cultivation etc.) factors are condensed into one parameter, r_e, which affects the decomposition rates of Y and O equally. The parameter r_e does not affect the 'humification coefficient' (h), i.e. the fraction of the outflux from Y that enters O. Note, however, that h can be set differently, not only depending on variation in litter quality but also depending on, e.g. clay content of the soil. All symbols are explained in Appendix A.

If carbon input to the soil is denoted as i and initial pools sizes are denoted Y_0 and O_0, respectively, the differential equations describing the state variable dynamics are:

$$\frac{\mathrm{d}}{\mathrm{d}t}Y = i - k_Y r_e Y, \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O = hk_Y r_e Y - k_O r_e O, \tag{2}$$

See Appendix B for the integrated forms of these equations.

2.2. ICBM/N

When modelling carbon fluxes in this way, only net fluxes are considered (Fig. 2, 'ICBM'). However, to model nitrogen fluxes as a function of carbon fluxes, we have to reconsider the outfluxes from Y (Fig. 2). Let e_y be the yield efficiency of the soil organism community (the fraction of the outflux from Y converted into biomass growth at each time step), k_g be the rate constant for gross carbon outfluxes from Y and h_g the fraction of this flux that is not respired and enters O. Note that h_g is different from h, which is the fraction of net carbon outfluxes from Y that enters O (Fig. 2). Then

$$\frac{\mathrm{d}}{\mathrm{d}t}Y = i + k_g r_e (\mathrm{e}_Y(1-h_g) - 1)Y, \tag{3}$$

describes the dynamics of carbon in Y. Let CO_2–C evolution from Y and the flux from Y to O be equal in Eq. (1) and Eq. (3), i.e. $k_Y r_e (1-h)Y = k_g r_e (1-e_Y)Y$ and $k_Y r_e h Y = k_g r_e e_Y h_g Y$ (cf. Fig. 2); then

$$k_g = k_Y \frac{1-h}{1-e_Y}, \tag{4}$$

and

$$h_g = h\frac{1-e_Y}{e_Y(1-h)}. \tag{5}$$

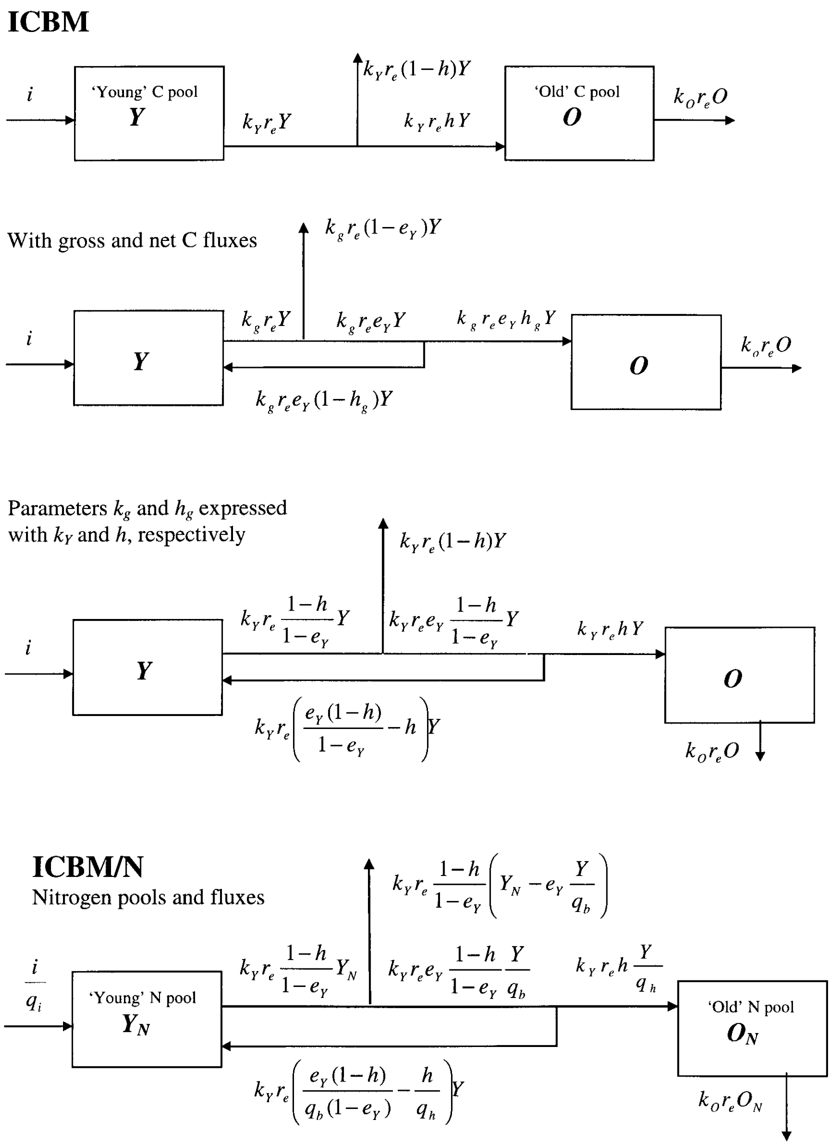

Fig. 2. Structure of the ICBM/N model. The derivation of 'N pools and fluxes' from carbon fluxes 'ICBM'. 'Step 1' and 'Step 2' are intermediate stages in model development. Flux equations are positioned close to their respective arrows. See text and parameter list (Appendix A) for definitions of variables and parameters.

Inserting Eq. (4) and Eq. (5) into Eq. (3) gives (see Fig. 2):

$$\frac{\mathrm{d}}{\mathrm{d}t}Y = i + k_Y r_e \left(\frac{(1-h)(e_Y - 1)}{(1-e_Y)} - h\right) Y. \tag{6}$$

Let the C:N ratios of input and of soil organism biomass be denoted by q_i and q_b, respectively. Then the corresponding differential equations describing nitrogen dynamics (index N) become (Fig. 2, ICBM/N):

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{\mathrm{N}} = \frac{i}{q_i} + k_Y r_e \left(\frac{e_Y(1-h)}{q_b(1-e_Y)} - \frac{h}{q_h}\right) Y - k_Y r_e \frac{1-h}{1-e_Y} Y_{\mathrm{N}}, \tag{7}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O_{\mathrm{N}} = k_Y r_e h \frac{Y}{q_h} - k_O r_e O_{\mathrm{N}}. \tag{8}$$

See also Appendix A for parameter descriptions and Appendix B for the integrated forms of the equations.

2.3. ICBM/2

The ICBM model can easily be extended to include several Y- and O-pools. Let i consist of different qualities with respect to decomposability and C:N ratios. Then, e.g. for two Y-pools (one 'labile' and one 'refractory') and one O-pool, the dynamics of carbon can be described with the equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_l = i_l + k_l r_e Y_l, \tag{9}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_r = i_r + k_r r_e Y_r, \tag{10}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O_2 = r_e h(k_l Y_l + k_r Y_r) - k_O r_e O_2. \tag{11}$$

2.4. ICBM/2N

The nitrogen dynamics can then be described by the equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{\mathrm{N}l} = \frac{i_l}{q_{il}} + k_l r_e \left(\frac{e_l(1-h)}{q_b(1-e_l)} - \frac{h}{q_h}\right) Y_l - k_l r_e \frac{1-h}{1-e_l} Y_{\mathrm{N}l}, \tag{12}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{\mathrm{N}r} = \frac{i_r}{q_{ir}} + k_r r_e \left(\frac{e_r(1-h)}{q_b(1-e_r)} - \frac{h}{q_h}\right) Y_r - k_r r_e \frac{1-h}{1-e_r} Y_{\mathrm{N}r}, \tag{13}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O_{2\mathrm{N}} = \frac{r_e h}{q_h}(k_l Y_l + k_r Y_r) - k_O r_e O_{2\mathrm{N}}. \tag{14}$$

In Eqs. (12)–(14), we assumed that h and q_h are equal for both Y-pools. Naturally, these parameters can also be set to different values for each pool, but this requires more parameters and some additional algebra. See also Appendix for parameter descriptions and integrated forms of equations.

2.5. ICBM/2B

So far we have assumed that microbial biomass is an implicit part of the Y-pool(s), i.e. microbial biomass is assumed to be in steady-state. In cases when this assumption is not valid, i.e. microbial growth and mortality are not equal, microbial biomass has to be expressed explicitly. This can be the case when environmental conditions and/or input rates are changed, e.g. due to changes in land use or seasonal changes (e.g. Hansson et al., 1990; Kandeler et al., 1999).

Further, estimates of microbial biomass C and N, obtained using chloroform fumigation methods are commonly used (Powlson, 1994), i.e. data are often available. Therefore, we also devised a model where microbial biomass is explicitly modelled (Figs. 1 and 3).

Let the substrate/soil C consist of two 'Young' (Y_{lB} and Y_{rB} as in ICBM/2) and an 'Old' (O_B) pool. A fraction (e_l) of the outflux from Y_{lB} available at each time step is used for biomass growth and incorporated into microbial biomass (B). A fraction (h_r) of the outflux from Y_{rB} available at each time step is humified directly without being assimilated by organisms, and a fraction ($(1-h_r)e_r$) is used for biomass growth and incorporated into microbial biomass (B). Let, further, the mortality rate of B be k_m. A fraction (h_m) of the outflux from B is humified and incorporated into O_B, and the remaining amount is recycled to B or lost as CO_2. A fraction (e_O) of the outflux from O_B is used for biomass growth and incorporated into B. Then, the dynamics of the system can be described by the equations (cf. Fig. 3):

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{lB} = i_r - k_l r_e Y_{0lB}, \tag{15}$$

$$\frac{d}{dt}Y_{rB} = i_r - k_r r_e Y_{0rB}, \tag{16}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}B = a_{11}B + a_{12}O_B + b_{11} + b_{12}\mathrm{e}^{-k_r r_e t} + b_{13} + b_{14}\mathrm{e}^{-k_l r_e t}, \tag{17}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O_B = a_{21}B + a_{22}O_B + b_{21} + b_{22}\mathrm{e}^{-k_r r_e t}, \tag{18}$$

where a_i and b_j are combinations of parameters and initial values as denoted in Appendix B.

2.6. ICBM/2BN

Assuming that the C:N ratio of the organism biomass does not change with time, the corresponding dynamic equations for nitrogen become

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{\mathrm{N}lB} = \frac{i_l}{q_{il}} - k_l r_e Y_{\mathrm{N}lB}, \tag{19}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}Y_{\mathrm{N}rB} = \frac{i_r}{q_{ir}} - k_r r_e Y_{\mathrm{N}rB}, \tag{20}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}B_{\mathrm{N}} = \frac{dB}{dt}\frac{1}{q_b}, \tag{21}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}O_{\mathrm{N}B} = k_m r_e h_m \frac{B}{q_m} + k_r h_r \frac{Y_r}{q_r} - k_O r_e O_{\mathrm{N}B}. \tag{22}$$

See Appendix B for the analytical solutions of these equations.

3. Statistical analysis and optimisation techniques

The models were fitted to data using non-linear regression analysis (procedure NLIN in SAS (SAS, 1985, SAS Institute Inc., NC)) by the multivariate secant method (Ralston and Jennrich, 1979), which was used when optimising pre-selected parameter values to measured data.

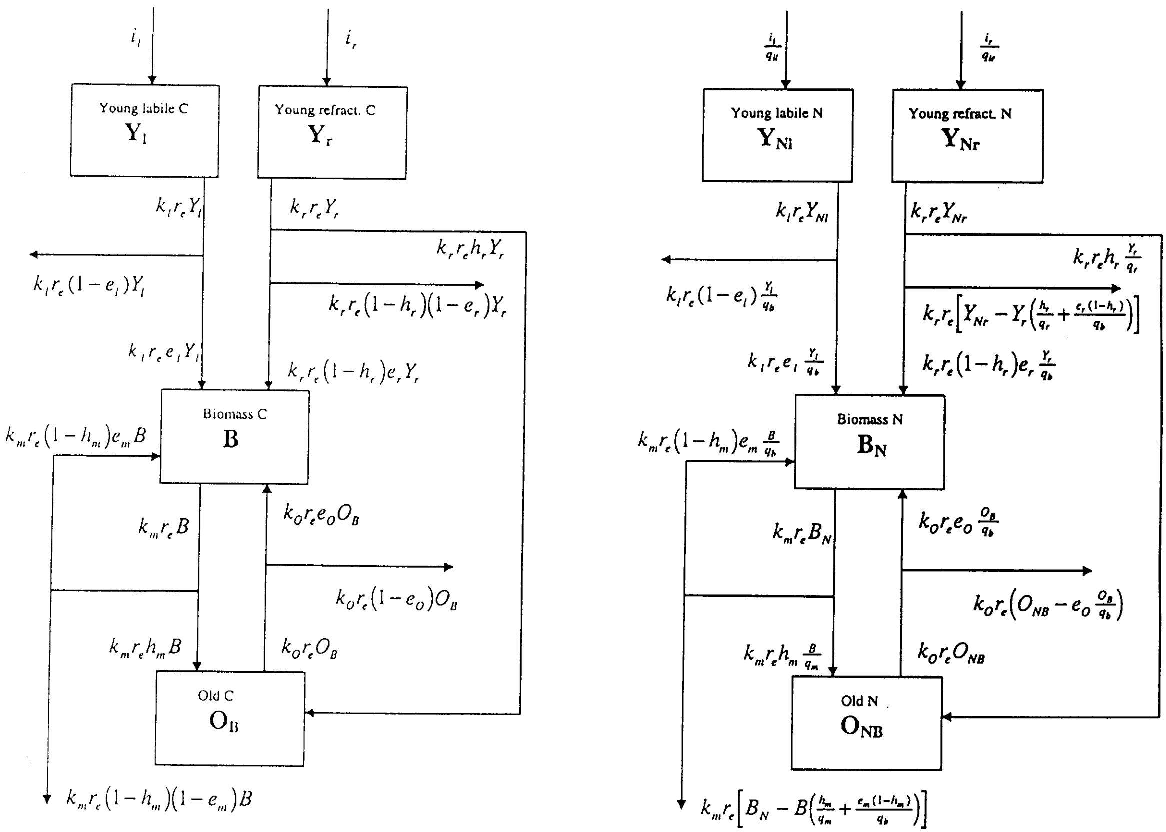

Fig. 3. Structure (pools and fluxes) of the ICBM/2BN model. Flux equations are positioned close to their respective arrows. See text and parameter list (Appendix A) for definitions of variables and parameters.

4. Application examples

4.1. Application of ICBM/N to a long-term field experiment

The ICBM/N model was fitted to the top-soil (0–23 cm) of the treatment of the Hoosfield Continuous Barley experiment (Jenkinson and Johnston, 1977), where farmyard manure (FYM) is added annually. Firstly, Eq. (A1) and Eq. (A2) were fit to the data for soil carbon stocks by optimising k_Y and k_O simultaneously using non-linear regression (the unit for t was year). Thereafter, Eq. (A6) and Eq. (A7) were fitted to the data for soil nitrogen stocks by optimising e_Y. All other parameter values were taken from measurements or estimated outside the model: The amounts of C and N annually applied as FYM were 0.3 and 0.0225 kg m^{-2} (Jenkinson and Rayner, 1977). The annual input from above- and below-ground litter was not given, but we assumed them to be 0.17 kg C and 0.0025 kg N m^{-2} (see Kätterer and Andrén, 1999). Thus, the weighted C:N ratio of the input, q_i, was $(0.3+0.17)/(0.0225+0.0025)=18.8$.

Correspondingly, the humification quotient, $h=0.243$, was the weighted mean relative to the amount of input via FYM ($h_{\mathrm{man}}=0.31$) or crop residues ($h_{\mathrm{crop}}=0.125$). Parameter values for h_{man} and h_{crop} were taken from Andrén and Kätterer (1997). Initial amounts of soil C and N were 3.07 and 0.341 kg m^{-2}, respectively. We assumed 0.3 kg C and 0.075 kg N m^{-2} to be easily decomposable, i.e. Y_0 and Y_{0N}. The C:N ratio of decomposers was assumed to be equal to 5. The resulting R^2-values were 0.92 and 0.81 for C and N, respectively (Fig. 4). All parameter values used to produce Fig. 4 are presented in Table 1.

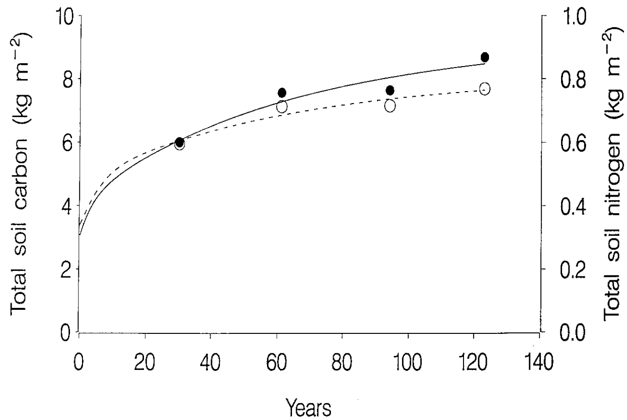

Fig. 4. Measured (symbols) and modelled (lines) dynamics of soil carbon (●; ——) and nitrogen (○; -----) stocks in one treatment in Hoosfield Continuous Barley experiment where farmyard manure was applied annually (Jenkinson and Johnston, 1977). See Table 1 for initial and parameter values.

4.2. Short-term application of ICBM/2N (biomass implicitly expressed)

The ICBM/2N model was applied to data for two treatments in an incubation experiment (Jansson, 1958). The incubated soil samples were from 'Nåntuna', a sandy clay loam in central Sweden (31% clay, 2.56% organic C, 0.252% organic N, pH (H_2O) 5.1). Samples of about 100 g dry soil were incubated at 100% WHC for 66 days. At the start of the incubations at about 20°C, ammonium sulphate was added in both treatments. In one treatment, '-straw', no organic amendments were added and in the other treatment, winter wheat straw was added corresponding to 4.070 mg C and 0.0348 mg N g per dry soil (Table 1).

For this model application, we assumed the same h-value for straw as in the long-term application ($h=0.125$). The evolution of carbon dioxide carbon (CO_2–C) was estimated by fitting the difference between initial C amounts in the soil and Eqs. (A11) and (A12) and Eq. (A15) simultaneously to both treatments:

$$CO_2(t)=Y_{0l}+Y_{0r}+O_0-Y_l(t)-Y_r(t)-O_2(t). \tag{23}$$

Values for k_l, k_r, and k_O were estimated simultaneously. Input, i, was zero and r_e was set to unity. The initial value for Y_l was the carbon amount added as straw. The distribution of the initial amounts of C in the soil (25.60 mg g per dry soil) between Y_r and O_2 was the fourth parameter, which was optimised simultaneously in this procedure. The resulting cumulative C evolution is shown in Fig. 5.

The parameter values as estimated for C dynamics (ICBM/2) were used when modelling nitrogen mineralisation/immobilisation (ICBM/2N). Three further parameters relating to N dynamics had to be set, i.e. the yield efficiency (e_r), the C:N ratio of micro-organisms (q_b) and the initial distribution of N between Y_{Nr} and O_{2N}. We assumed q_b to be 5, and the remaining two parameters were estimated by optimisation. The initial amount of N in Y_{Nl} was set to the amount of N added in straw. Since i was zero, the value of the state variables at steady-state also equalled zero.

The resulting dynamics of soil mineral nitrogen (N_{min}) is then equal to the difference between the initial total amount of N in the soil and Eqs. (A18) and (A19) and Eq. (A24):

$$N_{min}(t) = N_{0min} + Y_{0Nl} + Y_{0Nr} + O_{0N} - Y_{Nl}(t) - Y_{Nr}(t) - O_{2N}(t), \tag{24}$$

where N_{0min} is the initial amount of mineral N in the soil. The resulting R^2-values were 0.99 and 0.94 for C and N, respectively (Fig. 5; see Table 1 for parameter values).

Table 1
Initial amounts of carbon and nitrogen and parameter values for the model applications[a]

Symbol	lt	mt	st−s	st+s	st_b
Initial values of state variables					
B_0	–	–	–	–	0.109
O_0	2.77	0	25.2	25.2	21.67
O_{0N}	0.334	0	2.485	2.485	2.00
Y_0	0.3	–	–	–	–
Y_{0l}	–	12.3	0	4.07	–
Y_{0r}	–	437.7	0.39	0.39	0.22
Y_{0N}	0.0075	–	–	–	–
Y_{0Nl}	–	2.6	0	0.0348	–
Y_{0Nr}	–	3.5	0.035	0.035	0.066
Parameter values					
e_Y	0.362	–	–	–	–
e_l	–	0.0715	–	0.287	–
e_r	–	0.0715	0.287	0.287	0.6
e_O	–	–	–	–	0.3
e_m	–	–	–	–	0.6
h	0.243	0.1	0.125	0.125	–
h_m	–	–	–	–	0.1
h_r	–	–	–	–	0
i	0.47	0	0	0	0
k_l	–	15	–	0.015	–
k_m	–	–	–	–	0.1
k_O	0.0154	0.0001	0.000098	0.000098	0.00061
k_r	–	0.0105	0.0848	0.0848	0.5
k_Y	0.259	–	–	–	–
q_b	5	5	5	5	3.32
q_h	11.75	12	10	10	–
q_i	18.8	–	–	–	–
q_m	–	–	–	–	10
r_e	1	*	1	1	1

[a] 'long-term' (lt),'medium-term' (mt),'short-term -straw' (st−s),'short-term +straw' (st+s) and 'short-term, biomass explicit' (st_b). Mass units for 'lt' were kg m^{-2} and mg g^{-1} dry soil in the other applications.
* used as a driving variable (see text).

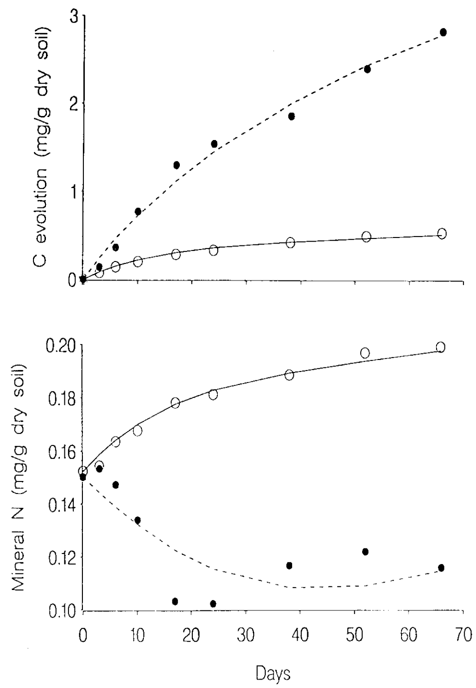

Fig. 5. Measured (symbols) and modelled (lines) dynamics of accumulated CO_2-C evolution and nitrogen mineralisation/immobilisation from the Nåntuna soil as incubated at about 20°C (Jansson, 1958). Treatments were: with straw (●; -----) and without straw (○; ——). See Table 1 for initial and parameter values.

4.3. Short-term application of ICBM/2BN (microbial biomass explicitly expressed)

The ICBM/2BN model was applied to data from a Japanese upland soil (Azmal et al., 1996) but with the parameters set to only use one Y pool (ICBM/BN). After a preincubation at 20°C, soil samples (clay loam; 20.5% clay; pH(H_2O) 5.6; 2.2% C; 0.21% N), corresponding to 20 g dry soil, were incubated at 35°C during eight weeks. The control treatment is considered here. CO_2–C evolution and soil mineral N were sampled nine times during the incubation period and microbial biomass C and N were estimated using the chloroform-extraction method. At the start of the incubation, the measured amount of C in microbial biomass was 0.109 mg g^{-1} dry soil (Table 1). Of the total initial amount of C in the soil (22 mg g per soil), 0.22 mg was assumed to be 'Young' (Y_{0rB}). Thus, O_{0B} was 21.67 mg. The initial amounts of soil mineral N (0.238 mg) and of total organic N (2.1 mg) were given. The allocation of organic N between the three pools considered here was based on the assumption that the ratios Y_{0r}/Y_{0Nr} and B_0/B_{0N} were equal to q_b, i.e. the mean C/N ratio in microorganisms as measured during the experiment. The mortality rate of organisms (k_m) was assumed to be equal to 0.1 per day. Parameter h_m was set to 0.1 and k_r was set to an arbitrary high value (0.5 per day). The value of e_O was set to 0.3 and parameters e_m and e_r, which were assumed to equal, were set to 0.6. The remaining parameter k_O was estimated by least square fitting. The resulting C and N dynamics are shown in Fig. 6.

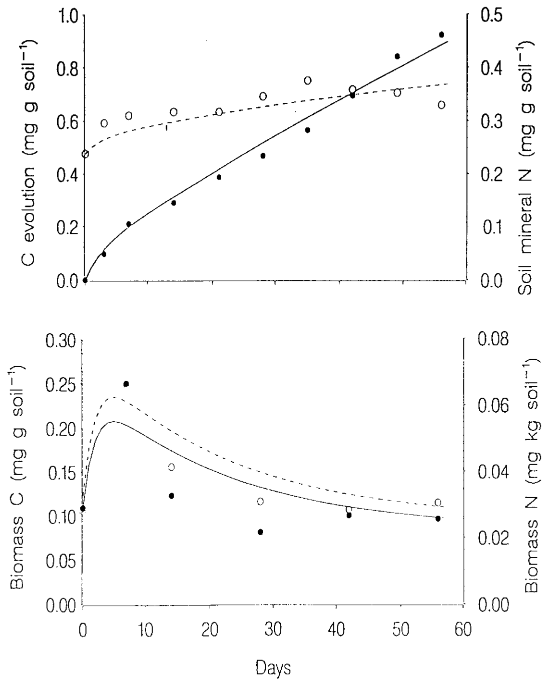

Fig. 6. Measured (symbols) and modelled (lines) dynamics of accumulated CO_2-C evolution (●; ——), mineral N (○; -----) and carbon (●; ——) and nitrogen (○; -----) in microbial biomass in soil samples (control treatment) incubated at 35°C (Azmal et al., 1996). See Table 1 for initial and parameter values.

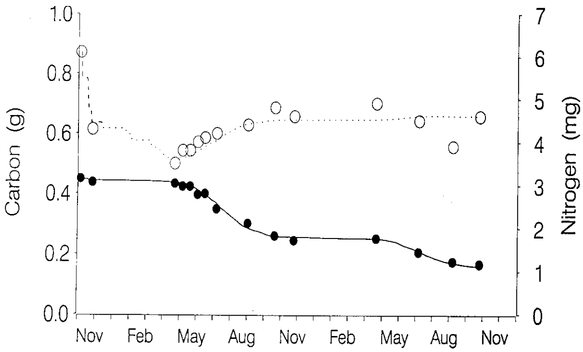

Fig. 7. Measured (symbols) and modelled (lines) dynamics of carbon (●; ——) and nitrogen (○; -----) in decomposing straw (Andrén and Paustian, 1987). See Table 1 for initial and parameter values.

4.4. Application of ICBM/2N to a medium-term experiment, transformation of time

The ICBM/2N model was applied to data derived from a litter-bag experiment (Andrén and Paustian, 1987), where barley straw was incubated in litter bags at 10–15 cm depth in an experimental field, Kjettslinge, in central Sweden (Fig. 7; Table 1). Remaining mass and nitrogen content were sampled at 14 occasions during a two-year period and daily soil temperature and moisture driving variables were available. A constant C concentration of 45% was assumed here. As in the short-term application, i was equal to zero, and thus, the state equations condensed to much simpler expressions. The values of e_l and e_r were assumed to be equal. To incorporate the effects of climate on decomposition rates, the independent variable t was transformed. We calculated daily values for parameter r_e as function of soil temperature (T) and soil water tension (Ψ):

$$r_e(\Psi,\ T) = F_\Psi F_T, \tag{25}$$

where moisture influence was assumed to be a log-linear function of soil water potential (Ψ):

$$F_\Psi = \begin{cases} 1 & \text{for } \Psi > \Psi_{max} \\ \dfrac{\log(\Psi_{min}/\Psi)}{\log(\Psi_{min}/\Psi_{max})} & \text{for } \Psi_{min} < \Psi < \Psi_{max} \\ 0 & \text{for } \Psi < \Psi_{min} \end{cases} \tag{26}$$

where Ψ is the soil water potential (MPa) and Ψ_{max} and Ψ_{min} are boundary values for maximum and minimum water potentials (Andrén and Paustian, 1987). Here, Ψ_{max} and Ψ_{min} were set to -1.5 and 0.005 MPa, respectively.

The dependence of decomposition rates on soil temperature was calculated according to a function proposed by Ratkowsky et al. (1982), which we normalised for 23°C, the maximum soil temperature measured in the field:

$$F_T = \frac{(T - T_{min})^2}{(23 - T_{min})^2}, \tag{27}$$

where T_{min} is the critical temperature at which $F_T = 0$. At lower temperatures F_T remains at zero. Here, T_{min} was set to -4°C.

The resulting daily values for $r_e(\Psi, T)$ were summed over the experimental period, i.e. 721 days. When applying the model to the data, in analogy with the use of temperature sums, we replaced t as the independent variable with t_r, i.e. the 'climate sum':

$$t_r = \sum_{t=1}^{t} r_e(\Psi, T). \tag{28}$$

Initial values for Y_l and Y_{Nl} were set to the measured amount of water-soluble C and N that was lost during the first sampling interval, i.e. 12.3 and 2.6 mg C and N, respectively (Andrén and Paustian, 1987). The remaining initial amounts of C (437.7 mg) and N (4.3 mg) were assumed to be Y_{0r} and Y_{0Nr}, respectively. O_{02} and O_{0N2} were assumed to be equal to zero. Values for h and q_b were set to 0.1 and 10, respectively. The rate constants k_l and k_O were set to arbitraryly high (15) and low (0.0001) values. These two parameters had little influence on the dynamics here, since almost all C was in Y_r. The model equations were fitted to the carbon data by optimising k_r, and to the nitrogen data by optimising e_r (Fig. 7; Table 1). The resulting R^2-values were 0.99 and 0.88 for C and N, respectively.

5. Conclusions

The models devised here, when presented as box-and-arrow diagrams, represent more or less the conventional wisdom of soil C and N modelling. They are similar to those implemented in many soil organic matter models and decomposition sub-model in complex ecosystem models, e.g. Van Dijk et al. (1985), Jenkinson et al. (1987), Johnsson et al. (1987), Parton et al. (1987), Hansen et al. (1991), Bradbury et al., 1993). First-order assumptions, the divisions into a number of pools, and subsequent simulations have a long history (see, e.g. Tenney and Waksman, 1929; Flanagan and Bunnell, 1975; Paustian et al., 1997). Given this background, it is not surprising that the here presented models could be parameterised for a set of widely different applications. A relevant question may therefore be: Have we only been curve-fitting and not really gained any new insights? In answer to this we can point out that coarse curve-fitting is not a property of the models, but instead of the application. For a deeper analysis of the applications, more sophisticated methods, such as inverse modelling (e.g. Abbaspour et al., 1997), are available to condition parameter values to one or several measured variables simultaneously (Abbaspour et al., 1999).

Most of the conceptual pools in all current soil organic matter models do not correspond directly with experimentally measurable fractions (Powlson, 1996), but a reasonable correspondence can be expected between, e.g. chloroform fumigation and true ‘microbial biomass’. This is also true for the models presented here, but their simplicity reduces this problem, since parameter values can be estimated simultaneously for different treatments as demonstrated here as well as for larger data sets (cv. Kätterer and Andrén, 1999).

When estimating several parameters simultaneously as we did for the short-term (biomass implicit) example using ICBM/2N, some parameters may be highly correlated. In our example, k_r, k_O and the distribution of initial carbon between Y_r and O were highly correlated ($|r > 0.9|$). This implies that changes in the values of one parameter can be compensated by changes of the other two. Setting one of these three parameters to values that were 50% higher or lower than their originally optimised estimates and re-running the optimisation program resulted in new parameter values whereas R^2-values were affected only marginally (< 3%). When applying to large data sets, this correlation probably will decline. However, it is finally up to the scientist to select the most reasonable combination of parameter values — the here presented framework of models will facilitate this work.

A set of functions can be developed, with which a reasonable parameter set can be constructed more or less automatically based on soil type, climatic zone data, primary productivity, management practices, etc. (see e.g. Franko et al., 1995, 1996). Calibrated from long-term field experiments, predictions regarding management implications on long-term soil fertility can be made, and, calibrated from decomposition experiments, predictions regarding carbon and nitrogen balances can be performed. Thus, the models can be used for analysing laboratory experiments (see e.g. Kätterer et al., 1998; Lomander et al., 1998) as well as being included in management-related software, e.g. to estimate fertiliser inputs and regional carbon balance- and land use change modelling.

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Appendix A

Constants and parameters used in the ICBM family of models. Symbols, typical dimensions and description. Mnemonically useful words underlined; initial values have index 0, zero. Note that the initial constants and parameters used in the carbon sub-models are re-used in the carbon/nitrogen models. See Fig. 1 for model structures

One 'Young' pool

ICBM — *two initial state variable values, five parameters*

Y_0	kg	Initial C mass of the 'Young' pool
O_0	kg	Initial C mass of the 'Old' pool
i	kg per year	Annual C input to soil
k_Y	Per year	Decomposition rate constant for the 'Young' pool
k_O	Per year	Decomposition rate constant for the 'Old' pool
h	Dimensionless	'Humification coefficient'; fraction of 'Young' outflux that enters 'Old'
r_e	Dimensionless	External response factor that affects outflux from 'Young' and 'Old'

ICBM/N — *four initial values, nine parameters (incl. ICBM)*

$Y_{0\mathrm{N}}$	kg	Initial N mass of the 'Young' pool
$O_{0\mathrm{N}}$	kg	Initial N mass of the 'Old' pool
q_i	Dimensionless	quality, C/N ratio of input, I
q_b	Dimensionless	C/N ratio of soil organism biomass
q_h	Dimensionless	C/N ratio of 'humification'; the influx to O
e_Y	Dimensionless	efficiency, i.e. the fraction of C flux from Y allocated to organism growth

Two 'Young' pools

ICBM/2 — *three initial values, seven parameters*

Y_{0l}	kg	Initial C mass of the 'Young and labile' pool, replaces Y_0 ($Y_{0l}+Y_{0r}=Y_0$)
Y_{0r}	kg	Initial C mass of the 'Young and refractory' pool, replaces Y_0
O_0	kg	Initial C mass of the 'Old' pool
i_l	kg per year	Annual C input to soil, labile part
i_r	kg per year	Annual C input to soil, refractory part
k_l	Per year	Decomposition rate constant, 'Young and labile' pool, replaces k_y
k_r	Per year	Decomposition rate constant, 'Young and refractory' pool, replaces k_y
k_O	Per year	Decomposition rate constant for the 'Old' pool
h	Dimensionless	'Humification coefficient'; fraction of 'Young' outflux that enters 'Old'
r_e	Dimensionless	External response factor that affects outflux from 'Young' and 'Old'

ICBM/2N — *six initial values, 13 parameters (incl. ICBM/2)*

$Y_{0\mathrm{N}l}$	kg	Initial N mass of the 'Young and labile' pool
$Y_{0\mathrm{N}r}$	kg	Initial N mass of the 'Young and refractory' pool
$O_{0\mathrm{N}}$	kg	Initial N mass of the 'Old' pool
q_{il}	Dimensionless	C/N ratio of labile input
q_{ir}	Dimensionless	C/N ratio of refractory input
q_b	Dimensionless	C/N ratio of soil organism biomass
q_h	Dimensionless	C/N ratio of 'humification'; the influx to O
e_l	Dimensionless	efficiency, i.e. the fraction of C flux from Y_l allocated to organism growth
e_r	Dimensionless	efficiency, i.e. the fraction of C flux from Y_r allocated to organism growth

Two 'Young' pools and microbial biomass

ICBM/2B — *four initial values, 13 parameters*

Y_{0lB}	kg	Initial C mass of the 'Young and labile' pool, defined for Biomass model
Y_{0rB}	kg	Initial C mass of the 'Young and refractory' pool, defined for Biomass model
B_0	kg	Initial Biomass C of soil organisms

O_{0B}	kg	Initial C mass of the 'Old' pool, defined for Biomass model
i_l	kg per year	Annual C input to soil, refractory part
i_r	kg per year	Annual C input to soil, labile part
k_l	Per year	Decomposition rate constant, 'Young and labile' pool
k_r	Per year	Decomposition rate constant, 'Young and refractory' pool
k_m	Dimensionless	mortality rate of organism biomass
k_O	Per year	Decomposition rate constant for the 'Old' pool
h_m	Dimensionless	'Humification coefficient'; fraction of organism mortality that enters 'Old'
h_r	Dimensionless	'Humification coefficient'; fraction of 'Young and refractory' outflux to 'Old'
r_e	Dimensionless	External response factor that affects outflux from 'Young' and 'Old'
e_l	Dimensionless	efficiency, i.e. the fraction of C flux from Y_l allocated to organism growth
e_r	Dimensionless	efficiency, i.e. the fraction of C flux from Y_r allocated to organism growth
e_m	Dimensionless	efficiency, i.e. the fraction of organism mortality C allocated to organism growth
e_O	Dimensionless	efficiency, i.e. the fraction of C flux from Old allocated to organism growth

ICBM/2BN — *eight initial values, 18 parameters (incl. ICBM/2B)*

$Y_{0Nl/B}$	kg	Initial N mass of the 'Young and labile' pool, defined for Biomass model
$Y_{0\mathrm{Ni}}$	kg	Initial N mass of the 'Young and refractory' pool, defined for Biomass model
O_{0NB}	kg	Initial N mass of the 'Old' pool, defined for Biomass model
q_{il}	Dimensionless	C/N ratio of labile input
q_{ir}	Dimensionless	C/N ratio of refractory input
q_b	Dimensionless	C/N ratio of soil organism biomass
q_m	Dimensionless	C/N ratio of mortality; flux from B to O.
q_r	Dimensionless	C/N ratio of direct flow from 'refractory and Young' to Old

Appendix B

Integrated forms of the model equations.

B.1. ICBM

On integration Eq. (1) and Eq. (2) in the article text become:

$$Y(t) = Y\mathrm{ss} + (Y_0 - Y\mathrm{ss})\mathrm{e}^{-k_Y r_e t}, \tag{A1}$$

$$O(t) = O\mathrm{ss} + (O_0 - O\mathrm{ss} - \phi)\mathrm{e}^{-k_O r_e t} + \phi\,\mathrm{e}^{-k_Y r_e t}, \tag{A2}$$

where

$$\phi = h\frac{k_Y r_e Y_0 - i}{(k_O - k_Y)r_e}, \tag{A3}$$

and Yss and Oss are the C pools at steady state:

$$Y\mathrm{ss} = \frac{i}{k_Y r_e}, \tag{A4}$$

$$O\mathrm{ss} = h\frac{i}{k_O r_e}. \tag{A5}$$

B.2. ICBM/N

On integration Eq. (7) and Eq. (8) become:

$$Y_\mathrm{N}(t) = Y_\mathrm{N}\mathrm{ss} + \left(Y_{0\mathrm{N}} - Y_\mathrm{N}\mathrm{ss} - \frac{\eta}{e_Y - h}(Y_0 - Y\mathrm{ss})\right) \mathrm{e}^{(-k_Y r_e(1-h)/1-e_Y))t} + \frac{\eta}{e_Y - h}(Y_0 - Y\mathrm{ss})\,\mathrm{e}^{-k_Y r_e t}, \tag{A6}$$

$$O_{\mathrm{N}}(t) = O_{\mathrm{N}}\mathrm{ss} + \left(O_{0\mathrm{N}} - O_{\mathrm{N}}\mathrm{ss} - \frac{\phi}{q_h}\right)\mathrm{e}^{-k_O r_e t} + \frac{\phi}{q_h}\mathrm{e}^{-k_Y r_e t}, \tag{A7}$$

where

$$\eta = \frac{e_Y(1-h)}{q_b} - \frac{h(1-e_Y)}{q_h}, \tag{A8}$$

and $Y_{\mathrm{N}}\mathrm{ss}$ and $O_{\mathrm{N}}\mathrm{ss}$ are the N pools at steady state:

$$Y_{\mathrm{N}}\mathrm{ss} = \frac{i}{k_Y r_e(1-h)}\left(\frac{1-e_Y}{q_i} + \eta\right), \tag{A9}$$

$$O_{\mathrm{N}}\mathrm{ss} = \frac{O\mathrm{ss}}{q_h}. \tag{A10}$$

B.3. ICBM/2

On integration Eqs. (9) and (10) and Eq. (11) become:

$$Y_l(t) = Y_l\mathrm{ss} + (Y_{0l} - Y_l\mathrm{ss})\mathrm{e}^{-k_l r_e t}, \tag{A11}$$

$$Y_r(t) = Y_r\mathrm{ss} + (Y_{0r} - Y_r\mathrm{ss})\mathrm{e}^{-k_r r_e t}, \tag{A12}$$

where $Y_l\mathrm{ss}$ and $Y_r\mathrm{ss}$ are the pool sizes at steady state:

$$Y_l\mathrm{ss} = \frac{i_l}{k_l r_e}, \tag{A13}$$

$$Y_r\mathrm{ss} = \frac{i_r}{k_r r_e}, \tag{A14}$$

and

$$O_2(t) = O\mathrm{ss} + (O_0 - O\mathrm{ss} - \phi_l - \phi_r)\mathrm{e}^{-k_O r_e t} + \phi_l \mathrm{e}^{-k_l r_e t} + \phi_r \mathrm{e}^{-k_r r_e t}, \tag{A15}$$

where

$$\phi_l = h\,\frac{k_l r_e Y_{0l} - i_l}{(k_O - k_l) r_e}, \tag{A16}$$

$$\phi_r = h\,\frac{k_r r_e Y_{0r} - i_r}{(k_O - k_r) r_e}, \tag{A17}$$

and the sum of C input $(i_l + i_r)$ to Y_l and Y_r at each time step is equal to i.

B.4. ICBM/2N

Nitrogen dynamics can be described by integrating Eqs. (12)–(14):

$$Y_{\mathrm{N}l}(t) = Y_{\mathrm{N}l}\mathrm{ss} + \left(Y_{0\mathrm{N}l} - Y_{\mathrm{N}l}\mathrm{ss} - \frac{\eta_l}{e_l - h}(Y_{0l} - Y_l\mathrm{ss})\right) \mathrm{e}^{(-k_l r_e(1-h)/1-e_l))t} + \frac{\eta_l}{e_l - h}(Y_{0l} - Y_l\mathrm{ss})\,\mathrm{e}^{-k_l r_e t}, \tag{A18}$$

$$Y_{\mathrm{N}r}(t) = Y_{\mathrm{N}r}\mathrm{ss} + \left(Y_{0\mathrm{N}r} - Y_{\mathrm{N}r}\mathrm{ss} - \frac{\eta_r}{e_r - h}(Y_{0r} - Y_r\mathrm{ss})\right) \mathrm{e}^{(-k_r r_e(1-h)/1-e_r))t} + \frac{\eta_r}{e_r - h}(Y_{0r} - Y_r\mathrm{ss})\,\mathrm{e}^{-k_r r_e t}, \tag{A19}$$

where

$$\eta_l = \frac{e_l(1-h)}{q_b} - \frac{h(1-e_l)}{q_h}, \tag{A20}$$

$$\eta_r = \frac{e_r(1-h)}{q_b} - \frac{h(1-e_r)}{q_h}, \tag{A21}$$

and

$$Y_{\mathrm{N}l}\mathrm{ss} = \frac{i_l}{k_l r_e(1-h)}\left(\frac{1-e_l}{q_{il}} + \eta_l\right), \tag{A22}$$

$$Y_{\mathrm{N}r}\mathrm{ss} = \frac{i_r}{k_r r_e(1-h)}\left(\frac{1-e_r}{q_{ir}} + \eta_r\right), \tag{A23}$$

where q_{il} and q_{ir} are the C:N ratios of input to the corresponding pools, and

$$O_{2\mathrm{N}}(t) = O_{\mathrm{N}}\mathrm{ss} + \left(O_{0\mathrm{N}} - O_{\mathrm{N}}\mathrm{ss} - \frac{\phi_l + \phi_r}{q_h}\right)\mathrm{e}^{-k_O r_e t} + \frac{\phi_l}{q_h}\,\mathrm{e}^{-k_l r_e t} + \frac{\phi_r}{q_h}\,\mathrm{e}^{-k_r r_e t}. \tag{A24}$$

B.5. ICBM/2B

The coefficients a_i and b_j in Eqs. (17) and (18) are:

$$a_{11} = k_m r_e(e_m(1-h_m) - 1), \tag{A25}$$

$$a_{12} = k_O r_e e_O, \tag{A26}$$

$$a_{21} = k_m r_e h_m, \tag{A27}$$

$$a_{22} = -k_O r_e, \tag{A28}$$

$$b_{11} = e_r(1-h_r)i_r, \tag{A29}$$

$$b_{12} = e_r(1-h_r)(k_r r_e Y_{0rB} - i_r), \tag{A30}$$

$$b_{13} = e_l i_l, \tag{A31}$$

$$b_{14} = e_l(k_l r_e Y_{0lB} - i_l), \tag{A32}$$

$$b_{21} = h_r i_r\ , \tag{A33}$$

$$b_{22} = h_r(k_r r_e Y_{0rB} - i_r). \tag{A34}$$

If the characteristic roots $\lambda_{1,2}$ of the system (Eqs. (17) and (18))

$$\lambda_{1,2} = \frac{a_{11}+a_{22}}{2} \pm \sqrt{\left(\frac{a_{11}+a_{22}}{2}\right)^2 + a_{12}a_{21} - a_{11}a_{22}} \tag{A35}$$

are distinct and real, then

$$\xi_1 e^{\lambda_1 t} + \xi_2 e^{\lambda_2 t}, \tag{A36}$$

is the complementary function of B and

$$c_0 + c_1 e^{-k_r r_e t} + c_2 e^{-k_l r_e t}. \tag{A37}$$

is the particular integral. Thus:

$$B(t) = \xi_1 e^{\lambda_1 t} + \xi_2 e^{\lambda_2 t} + c_0 + c_1 e^{-k_r r_e t} + c_2 e^{-k_l r_e t} \tag{A38}$$

is the general solution for B, where

$$c_0 = \frac{a_{12}b_{21} - a_{22}(b_{11}+b_{13})}{a_{11}a_{22} - a_{12}a_{21}}, \tag{A39}$$

$$c_1 = \frac{a_{12}b_{22} - b_{12}(a_{22}+k_r r_e)}{(k_r r_e)^2 + (a_{11}+a_{22})k_r r_e + a_{11}a_{22} - a_{12}a_{21}}, \tag{A40}$$

$$c_2 = \frac{-b_{14}(a_{22}+k_l r_e)}{(k_l r_e)^2 + (a_{11}+a_{22})k_l r_e + a_{11}a_{22} - a_{12}a_{21}}, \tag{A41}$$

and

$$\xi_1 = B_0 - \xi_2 - c_0 - c_1 - c_2, \tag{A42}$$

$$\begin{aligned}\xi_2 = \frac{1}{\lambda_2 - \lambda_1} [&a_{12}O_0 + (a_{11}-\lambda_1)B_0 + \lambda_1 c_0 \\ &+ (\lambda_1 + k_r r_e)c_1 + (\lambda_1 + k_l r_e)c_2 + b_{11} + b_{12} \\ &+ b_{13} + b_{14}],\end{aligned} \tag{A43}$$

where B_0 is the initial values of B.

On integration $Y_{lB}(t)$, $Y_{rB}(t)$ and $O_B(t)$ become:

$$Y_{lB}(t) = \frac{i_l}{k_l r_e} + \left(Y_{0lB} - \frac{i_l}{k_l r_e}\right) e^{-k_l r_e t}, \tag{A44}$$

$$Y_{rB}(t) = \frac{i_r}{k_r r_e} + \left(Y_{0rB} - \frac{i_r}{k_r r_e}\right) e^{-k_r r_e t}, \tag{A45}$$

$$\begin{aligned}O_B(t) = \frac{1}{a_{12}} [&(\lambda_1 - a_{11})\xi_1 e^{\lambda_1 t} + (\lambda_2 - a_{11})\xi_2 e^{\lambda_2 t} \\ &- a_{11}c_0 - b_{11} - b_{13} \\ &- (c_1(k_r r_e + a_{11}) + b_{12})e^{-k_r r_e t} \\ &- (c_2(k_l r_e + a_{11}) + b_{14})e^{-k_l r_e t}].\end{aligned} \tag{A46}$$

B.6. ICBM/2BN

On integrating Eqs. (15)–(18), the nitrogen dynamics become:

$$Y_{NlB}(t) = \frac{i_l}{q_{il}k_l r_e} + \left(Y_{0NlB} - \frac{i_l}{q_{il}k_l r_e}\right) e^{-k_l r_e t}, \tag{A47}$$

$$Y_{NrB}(t) = \frac{i_r}{q_{ir}k_r r_e} + \left(Y_{0NrB} - \frac{i_r}{q_{ir}k_r r_e}\right) e^{-k_r r_e t}, \tag{A48}$$

$$B_N(t) = \frac{B(t)}{q_b}, \tag{A49}$$

$$\begin{aligned}&O_{NB}(t) \\ &= \xi_3 e^{-k_O r_e t} + \frac{h_m k_m}{q_m}\left[\frac{\xi_1}{\lambda_1 + k_O} e^{\lambda_1 t} + \frac{\xi_2}{\lambda_2 + k_O} e^{\lambda_2 t} \right.\\ &\quad \left. + \frac{c_0}{k_O} + \frac{c_2}{k_O - k_l} e^{-k_l r_e t}\right] \\ &+ \frac{1}{k_O - k_r}\left[\frac{h_m k_m c_1}{q_m} + \frac{h_r k_r}{q_r}\left(Y_{0NrB} - \frac{i_r}{k_r r_e}\right)\right] e^{-k_r r_e t} \\ &+ \frac{h_r i_r}{q_r k_O r_e},\end{aligned} \tag{A50}$$

where

$$\xi_3 = O_{0NB} - \frac{h_m k_m}{q_m}\left[\frac{\xi_1}{\lambda_1 + k_O} + \frac{\xi_2}{\lambda_2 + k_O} + \frac{c_0}{k_O} + \frac{c_2}{k_O - k_l}\right] - \frac{1}{k_O - k_r}\left[\frac{h_m k_m c_1}{q_m} + \frac{h_r k_r}{q_r}\left(Y_{0NrB} - \frac{i_r}{k_r r_e}\right)\right] - \frac{h_r i_r}{q_r k_O r_e}. \quad \text{(A51)}$$

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