BASGRA_N User Guide

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1 Introduction

- BASGRA_N is a new version of the BASGRA model for growth and overwintering of grasslands. The new model was developed to allow simulation of additional phenomena: (1) the impact of N-supply on the plants and their environment, (2) the dynamics of greenhouse gases in plants and soil, (3) the dynamics of cell-wall content and digestibility of leaves and stems.
- The new model simulates the carbon-, nitrogen- and water-cycles in the plant-soil system in some detail. The previous model, BASGRA2014, lacked the nitrogen cycle and only simulated carbon-processes in the plants, not the soil. So the main processes added to the previous model are simulation of C and N in the soil, and of N in the plants. The dynamics of cell/wall content and digestibility are simulated using simple empirical functions of phenological stage.
- We refer to the user guide of BASGRA2014 (downloadable from Van Oijen et al. 2015) for a description of all unchanged processes. The present user guide focuses on the new parts of the model. We begin by giving a summary overview of the changes, and then give more details of the new processes. This is followed by a section that lists the files that have changed (BASGRA is implemented as a collection of multiple FORTRAN- and R-files, only some of which were changed to produce BASGRA_N). Then a first evaluation of the new model is given and some key references. Finally, in an Appendix, details of the exact code changes in modified files are described.

2.1 New state variables and processes

- BASGRA2014 had 23 state variables, of which 13 referred to plant variables and 10 to environmental variables. BASGRA_N has one extra plant state variable (NSH, the amount of nitrogen in aboveground plant parts; g N m-2) and seven extra soil state variables representing mineral nitrogen plus C and N in three other soil pools: litter and two forms of organic matter differing in decomposition rate. This brings the total number of state variables in BASGRA_N to 31 (14 plant, 17 environment). Nitrogen in roots is not simulated as a state variable but as root carbon times a constant N-C ratio, and nitrogen in reserves is considered absent.
- The dynamics of the new plant state variable NSH are the net result of growth (incorporating N taken up from the soil and from remobilisation), senescence and harvesting. The dynamics of the seven new soil state variables are simulated in the same way as in the forest model BASFOR (Van Oijen et al. 2005). The pool sizes vary as a result of external inputs (fertilisation, deposition, fixation), decomposition, uptake by plants, and losses to the environment (leaching, gaseous emission).

2.2 New inputs

• BASGRA_N requires the same input variables as BASGA2014, plus two new ones. The weather variables are the same: daily time series of radiation, temperature, precipitation, wind speed and humidity. Also retained is the need to supply the time schedule of grass cutting. The two new input time series are for fertilisation and for atmospheric deposition, both expressed in g N m-2 d-1.

2.3 New outputs

• In principle, every variable simulated by BASGRA_N can be included in the list of output variables. But in the archived version of BASGRA_N, a limited number of output variables are specified. These include the 31 state variables as well as process rates and intermediate variables of all three cycles (C, N and water) and of cell-wall content

and digestibility. New outputs also include crude protein content and ash content, both of which are estimated as linear functions of shoot nitrogen content.

2.4 New parameters

• The total number of model parameters has increased from 81 in BAS-GRA2014 to 113 in BASGRA_N. The new parameters include initial constants for the new state variables, control coefficients for new processes, N-C ratios and relative death rates of roots and stubble.

3 Assumptions, processes, mechanisms

We first describe the N-processes in the plants, and then give a summary of C- and N-processes in the soil. The soil description will be kept short because most of the mechanisms can be found in other models, in particular BASFOR (Van Oijen et al. 2005). We conclude by describing the processes of change in cell-wall content and digestibility.

3.1 Simulation of N in the plants

3.1.1 Availability of N, the "N-source"

- At every time step, the availability of N to the plants is determined by the amount of soil mineral N (state variable NMIN; g N m-2), plus the amount of N that becomes available from within the shoots by remobilisation.
- N-remobilisation is calculated by comparing the amount of N actually present in the shoots (NSH) to the amount of N that we would have seen if N-C ratio followed the same exponential profile in the sward as light, starting from the maximum N-C value allowed by the model at the top (NCSHMAX). In the model, that "expected" amount of shoot N is called NSHK, which can be read as "the amount of N in shoots if the profile would follow the light extinction coefficient K". The formula for NSHK is the following:
- NSHK = CSH * NCSHMAX * (1-exp(-K*LAI))/(K*LAI),
- where CSH = CLV+CST, i.e. carbon in leaves plus stems. The term "CSH*NCSHMAX" is the maximum possible amount of shoot-N (maximum N-C ratio at all positions), and the final term is the fraction of

that maximum that is realised in an exponential profile with coefficient K.

- Often NSH > NSHK, and we assume that the excess nitrogen (NSH NSHK) becomes available for growth at a given time constant. That process is called remobilisation.
- NMIN is available for plant uptake, but not all of it at the same time: the maximum plant uptake rate of soil mineral nitrogen is calculated as NMIN divided by a given time constant. Apart from plant uptake, NMIN is also depleted by loss to the environment (leaching, emission), and it is replenished from decomposition of organic material and from external inputs in the form of deposition, fertilisation and/or fixation. This makes NMIN into a highly dynamic variable that never contains more than a small fraction of total soil N, but one that plays a key role in regulating plant processes.
- So in the model, the N-source available for growth is equal to the excess of shoot-N plus soil mineral N, both terms divided by their own time constant.

3.1.2 Requirement for N, the "N-sink"

• In all versions of BASGRA, allocation of carbon to shoot growth depends on the balance between C-availability (from photosynthesis and reserves) and C-demand by leaves and stems. We refer to the shoot demand for C as its "sink strength". In BASGRA_N, a small N-source reduces shoot sink strength, but does not affect the sink strength of other processes. The effect of a limiting N-source on the shoot sink (for growth in terms of carbon) is assumed to be proportional to the N-source divided by the product of shoot sink and a maximum shoot N-C ratio. The latter product can be viewed as the N-sink of the plants. So shoot carbon sink is proportional to the source-sink ratio for N. In yet other words, when the N-source is too low to support shoot growth at maximum nitrogen concentration, shoot growth rate is reduced proportionately. The proportionality factor is called 'fNgrowth' in the model.

3.1.3 Effects of N-limitation on other plant processes than growth

• Apart from influencing shoot sink strength and thereby allocation patterns, N-limitation does not have an immediate effect on plant light-use

efficiency because the Rubisco-content and N-C ratio of upper leaves (parameter RUBISC, g m-2 leaf; parameter NCSHMAX, g g-1) are assumed to be constant. There is, however, an immediate effect on tillering: the leaf appearance rate, which provides site for tillering, is also proportional to fNgrowth. Note, however, that all other plant processes will also, but indirectly, be affected in the long-run by any changes in allocation.

3.1.4 Dynamics of plant N-C ratios

- The overall N-C ratio of stems and leaves, NCSH, is considered variable in BASGRA_N. In contrast, the N-C ratio of roots is assumed to be constant, and that of reserves is assumed to be zero. Although NCSH is variable, it is not fluctuating strongly, despite the fact that three processes affect it. These processes are growth, senescence and harvesting. All three processes change NCSH by adding or removing tissue that is not at the average N-C ratio. We assume that (1) growth adds young material at a ratio higher than average, (2) harvesting removes tissue also at higher-than-average N-C ratio, while (3) senescence removes tissue at lower than average N-C ratio.
- Calculation of the N-C ratios at which the three processes proceed is based on the assumption that nitrogen concentration follows an exponential function of LAI, counting from the youngest leaves downward. So a very small amount of shoot growth would have the maximum N-C ratio (parameter NCSHMAX), and greater amounts of new shoot growth would have slightly lower N-C ratios. Likewise, the harvested material from a very small cut would have high N-C ratio whereas big cuts would have lower N-C ratio because older, lower-N tissue would be included in the harvest. The loss of N in senescence also adheres to the concept of an exponential aboveground profile of N, but the assumption is here that the lowest-N tissue dies first, so days with high senescence may have slightly greater losses of N per unit tissue than days with only minor senescence. All these calculations require us to estimate KN, the "extinction coefficient for N" in the sward profile.

3.1.5 Derivation of the N-extinction coefficient, KN

 Assuming that nitrogen follows an exponentially decreasing curve in the canopy, starting from a given maximum N-C ratio at the top (NC-SHMAX), we should in principle be able to calculate KN as a function

- of total aboveground leaf area (LAI) and nitrogen (NSH). However, as we show now, there is no analytical solution to this problem, so we developed a somewhat intricate approximating equation for KN.
- As a general observation, we can say that if NSH > NSHK, then KN must be less than K (nitrogen "extinguishes" less quickly than light does) and if NSH<NSHK then KN > K. More precisely, KN can be solved from the following equation, similar to the one for NSHK above but with a different exponential coefficient:
- NSH = CSH * NCSHMAX * (1-exp(-KN*LAI))/(KN*LAI).
- Unfortunately that equation cannot be solved analytically for KN, because of the exponential term. In other words, even if all terms apart from KN itself are known, we cannot directly find the value of KN. However, we can find an approximation to KN by replacing the exponential term by its third-order Taylor expansion around KN equal to zero:
- 1-exp(-KN*LAI) = (approximately) KN*LAI (KN^2*LAI^2)/2 + (KN^3*LAI^3)/6.
- Plugging that approximation into the equation for NSH gives a quadratic equation that can be solved:
- $NSH = CSH * NCSHMAX * (1 KN*LAI/2 + KN^2*LAI^2/6),$
- and the solution of this quadratic equation is:
- KN = (approximately) $(3/2 \pm 3*sqrt(1/4 (2/3)*(1-NSH/(CSH*NCSHMAX))))/LAI.NotethatNSH/(CSH*NCSHMAX)mustbelargerthan5/8toensurethan rootisarealnumber.TheapproximationforKNmayleadtoextremevaluesofKNwhenKN*LAIbecomeslarge, butwecanstrengthenitbyrespectinganupperbound(calledKNMAX)forKNdeexp(-KN*LAI)) < 1, we find that:$
- KN < KNMAX = CSH * NCSHMAX / (NSH * LAI)
- We now check the quality of the approximation for KN for two extreme values of NSH: NSH = CSH*NCSHMAX and NSH = NSHK. We begin with the first case where we have a uniform profile of N with an N-C ratio that is everywhere equal to NCSHMAX. In other words, KN should be zero. We check this by plugging "NSH=CSH*NCSHMAX" into our approximative equation for KN and find that it simplifies to:

- KN_(NSH uniform) = (approximately) $(3/2 \pm 3*sqrt(1/4))/LAI = (3/2 \pm 3/2)/LAI$, and this indeed simplifies to KN = 0 provided we choose the "minus" solution of the quadratic equation. From now on we assume that the minus solution is the correct one and tune NSH = NSHK. In that case we should find—if our approximative equation is any good—that KN is about equal to the light extinction coefficient K. So we plug the equation given above for NSHK in
- KN_(NSH=NSHK) = (approximately) $(3/2 3 * \operatorname{sqrt}(1/4 (2/3)*(1-(1-\exp(-K*LAI))/(K*LAI)))) / LAI$
- We checked this result in EXCEL for many values of K and LAI. For small values of K*LAI, the approximation is excellent. For large values of K*LAI the approximation becomes increasingly worse, but KN's upper bound (KN-MAX = CSH*NCSHMAX/(NSH*LAI)) then comes to the rescue: KNMAX becomes increasingly close to the light extinction coefficient K. We can see that as follows:
- $KN_{NSH=NSHK} < KNMAX_{NSH=NSHK} = CSH*NCSHMAX/(NSHK*LAI)$ = K / (1-exp(-K*LAI)),
- where the denominator of the ratio gets increasingly close to unity when K*LAI becomes big.
- So also for this very different case, the approximative equation for KN, with upper bound, works well.

3.1.6 KN: rule and role

- The previous paragraph showed how we derived an approximative equation for KN, and an upper bound for it. Taking everything together, we work with the following rule for KN in the model:
- If NSH/(CSH*NCSHMAX) >= 5/8 then KN is assumed equal to the negative-branch solution of the approximative quadratic equation or to KNMAX, whichever is smaller, and
- If NSH/(CSH*NCSHMAX) < 5/8 then KN is assumed equal to KN-MAX.
- The role of KN in the model is to make sure that the effects of growth, harvesting and senescence on NSH are calculated correctly. These processes increase or decrease shoot biomass, and the amount of N that is gained or lost should be consistent with the N-profile as measured

by KN. We only show how this is calculated for senescence, but fairly similar equations apply to the two other processes. Daily senescence removes an amount DLAI from the LAI. The amount of carbon lost is less than DLAI/LAI because we assume that stems do not senesce. And the fraction of nitrogen lost in the same process is even less than that because we assume that senescent tissue is at the lower end of the exponential profile of N-C ratio in the canopy. We calculate the fraction of NSH lost in senescence as 1 minus the fraction of N remaining in leaves (stems are disregarded), and for that calculation we use the "nitrogen extinction coefficient" KN. The fraction of leaf biomass remaining (i.e. not senescing) is (LAI-DLAI)/LAI. The fraction of leaf N in the corresponding part of the exponential curve is equal to:

- Fraction non-senescing leaf $N = (1-\exp(-KN*(LAI-DLAI))) / (1-\exp(-KN*LAI))$
- So our estimate for the fraction of leaf N lost in daily senescence is 1 minus that amount. We may need to correct that estimate because KN, after all, is only approximated and not exactly known. We ensure that the N-C ratio of the senescing leaf tissue is not so low that the remaining biomass has more than the maximum permitted N-C ratio, NCSHMAX:
- DNSH >= NSH NCSHMAX * (CSH-DLV),
- where DLV is the carbon loss from the shoot (i.e. dying leaves) in senescence. So in the model, we take the loss of shoot N in senescence, DNSH, to be the maximum of our profile-based estimate and the amount needed to ensure that NCSH <= NCSHMAX.

3.2 Simulation of N in the soil

• The simulation of carbon and nitrogen in the soil follows the scheme for carbon devised by Goudriaan (1990), which we extended with nitrogen dynamics. We distinguish three general pools in the soil: litter ("LITT"), organic matter with a fast turn-over rate ("SOMF"), and organic matter with a slow turn-over rate ("SOMS"). Each type of soil pool contains both C and N, and their ratios can vary to some extent. So there are six state variables called CLITT, CSOMF, CSOMS, NLITT, NSOMF, NSOMS. Shoot senescence contributes to LITT, at the N-C ratio of the senescing material, and root senescence contributes

to SOMF at the N-C ratio of the roots which is a constant. Furthermore there are continuously operating transformations from LITT to SOMF to SOMS, in each case with some of the C being lost as CO2 and some of the N being lost to the soil mineral pool NMIN.

3.3 Simulation of cell-wall content and digestibility

- Our submodel for cell-wall content and digestibility is intermediate in complexity between the models of Gustavsson et al. (1995) and that of Bonesmo & Bélanger (2002).
- We added a subroutine 'Digestibility' to plant.f90 that calculates cell-wall-content (g g-1 DM) and digestibility (dimensionless) of leaves and stems.
- The subroutine calculates cell-wall content of:
 - leaves
 - stems
 - shoot dry matter (DMSH = DMLV + DMST + DMRES)
 - total aboveground dry matter (DM = DMSH + DMSTUB)
- The subroutine calculates digestibility of:
 - leaves
 - stems
 - cell walls overall
 - shoot dry matter
 - total aboveground dry matter
- The algorithm assumes that all dry matter other than cell walls is fully digestible. Digestibility of cell walls decreases linearly with phenological state (PHEN). Leaves, stems and stubble have different cellwall fractions but cell-wall digestibility itself does not differ among the different plant components. The cell-wall contents of both leaves and stems increase linearly with phenological state and are generally higher in stems than in leaves. Cell-wall content of reserves is zero and of stubble 100%.

4 Implementation of BASGRA N

• BASGRA_N is implemented in the same way as BASGRA2014, in the form of eight FORTRAN files that define model structure and parameterisation, plus a number of R-files for running the model and analysing the results. In this section, we merely name the files that were changed, for more details see the Appendix on "Details of file changes"

4.1 FORTRAN files

- The eight FORTRAN files (with extension ".f90") are:
 - BASGRA.f90
 - environment.f90
 - parameters plant.f90
 - parameters site.f90
 - plant.f90
 - resources.f90
 - set_params.f90
 - soil.f90
- Three of these files (parameters_plant.f90, parameters_site.f90, set_params.f90), together with an ASCII-file (parameters.txt), set the parameter values of the model.
- The remaining five f90-files form the heart of the model, representing the processes. The state equations which define how the state variables are updated every time step and the output variables are defined in 'BASGRA.f90'. The file 'environment.f90' is identical to the previous model version and simulates meteorology. The file 'resources.f90', which simulates light absorption and evapotranspiration, is also essentially unchanged apart from minor tidying up of the code. The file 'soil.f90' has changed considerably to include representation of the soil C- and N-cycles as well as nitrogen deposition and fertilisation. The file 'plant.f90' has also changed much.

4.2 R-files

- BASGRA_N uses the same suite of R-files as BASGRA2014 does for running the model, analysing results and carrying out Bayesian calibration of parameter distributions. There are some minor changes in some of the files:
 - In the following files, calendars for fertilisation and deposition are introduced: 'BC_BASGRA_MCMC.R', 'BC_BASGRA_MCMC_init_general.R', 'BC_plot_outputs_data.R', 'initialise_BASGRA_general' and all the 'initialisation BASGRA...' files.
 - 'BC_BASGRA_MCMC_init_general.R' has also been tidied up (unused code removed).
 - In 'initialise_BASGRA_general', names and units of new output variables are added, and an error in the calculation of 'sumdata' was corrected (the column number has been changed from 2 to 4, i.e. the column with the data values).

5 Evaluation and outlook

• Preliminary tests with this version of BASRA_N suggest that the model works well. However, this has to be checked in greater detail. Moreover, there are various parts of BASGRA_N that may be oversimplifications requiring further model development.

5.1 Needs for further model testing

- The following processes may require closer attention:
 - Dynamics of root-shoot ratio. There may be many data on this variable, but we have not checked yet how it responds to N-supply in the model.
 - Full N-budgets with all processes of nitrogen import and export.
 Such budgets can be set-up for:
 - * the whole soil-plant system,
 - * soil,
 - * plants,
 - * above-ground biomass

5.2 Data needs

- With the introduction of the N-relations in plant and soil, the model has become more data hungry. So there are questions about the availability of data for:
 - N-concentration ranges in timothy
 - Time series of state variables
 - General patterns of response to N (e.g. root-shoot ratio responses)
 - Impact of fertilisation
 - Impact of mixing with N-fixers (clover)
 - Information on remobilisation of N from senescent material

5.3 Further model structural development

• The following parts of the model may be reconsidered.

5.3.1 LUE

- At present, there is no direct effect of the sward N status on light-use efficiency (LUE). We may wish to make the LUE dependent on fN-growth or, perhaps more plausibly, the N-C ratio of the shoot, NCSH. We may encounter problems with circularity if we make fNgrowth affect other processes, as it is calculated based on the *actual* total carbon growth rate of the plants, not the potential rate.
- If we choose to implement an effect of NCSH on LUE, then maybe the parameter RUBISC can be removed from the model and, in subroutine LUECO2TM, be replaced by a variable RUBISC, calculated as being directly proportional to NCSHMAX. Also in that LUE-subroutine, the light extinction coefficient K may be replaced by the nitrogen extinction coefficient KN although that is not fully consistent with the concepts on which the LUE-calculation is based. An alternative method would be to calculate LUE as before but modify it then as a function of fNgrowth or NCSH/NCSHMAX.

5.3.2 The new algorithm for calculating the nitrogen profile (KN)

• At present, KN is estimated by solving a quadratic equation (and also recognising an upper bound to KN). Another way of modeling this would be to use a loop in which we find iteratively the KN-value that

gives an estimated NSH value (let's call it "NSH(KN)") within a small error from the actual value of NSH in the model. That is perhaps not elegant and also computationally demanding. However, we can use one single iteration of that idea as follows:

- Estimate KN as we do now
- Use that estimated KN to calculate NSH(KN)
- Compare NSH(KN) to NSH. If NSH(KN) > NSH then we need to adjust our estimate of KN, i.e. increase KN somewhat. If NSH(KN) < NSH, then we need to decrease KN somewhat.

5.3.3 Nitrogen uptake

• At present N-uptake is not a function of root biomass (CRT) or rooting depth, based on the assumption that mineral N is very mobile in soils and will generally move to roots sufficiently fast (given a certain time constant) to meet plant N-demand, irrespective of root system size. This assumption needs to be tested.

5.3.4 Nitrogen in stems, leaves and stubble

- NCSH is often observed to decrease with increasing biomass. We need to check whether the model reproduces that phenomenon. The reduction of NCSH may be caused, partly or completely, by an increase in the stem fraction of biomass, as stems are known to often have lower N-C ratio than leaves. The nitrogen in stems and leaves is currently lumped in the variable NSH, so we may want to separate this into NST and NLV, both with their own variable N-C ratio. We also need to check carefully in such a new model version (and in the current one) that the way senescence in terms of nitrogen is calculated is consistent with the senescence equations for carbon.
- Another consideration is whether the model assumption of zero N in stubble is justified.

5.3.5 Nitrogen in roots

• We may want to check whether the nitrogen source-sink calculations are considering the roots appropriately. Root growth requires nitrogen at a constant N-C ratio. Is this taken into account correctly in the calculation of the "plant nitrogen sink strength"?

5.3.6 Dynamics of soil mineral nitrogen

• Currently, the model code includes a line that sets NMIN to zero whenever the simulations lead to a (possibly very small) negative value. This positiveness-constraint is not elegant and only introduced because of numerical errors in the solution of the model equations. However, we may want to remove the need for this artificial approach by reformulating the processes affecting NMIN rather than NMIN itself - to ensure that the N-balance in the calculations remains closed.

5.3.7 Possible simplifications

- The N-C ratio of shoot growth may not need to be calculated as a function of KN if we assume that all new growth proceeds at the maximum N-C ratio of NCSHMAX.
- The line in the calculation of nitrogen loss associated with harvesting, where we ensure that the N-remaining (the unharvested material) is not exceeding the maximum N-C ratio, NCSHMAX, may be superfluous because the N-C ratio of harvested material should always be more than average (i.e. more than NCSH), given that KN cannot be less than zero and that tissue is harvested starting from the high-N top.

5.3.8 New processes

• There may be a use for simulating the uptake of amino acids, rather than mineral N, from manure, as scientific interest in the dynamics of organic N seems to be increasing.

5.3.9 Comparison with other models

- We need to investigate more closely how BASGRA_N compares to other grassland models or crop models including nitrogen relations:
- SPACSYS
 - Wu et al. 2007
 - Wu et al. (incl. Bob Rees and Andy Whitmore) 2015
- CATIMO
- STICS
- GECROS (Yin)

6 References

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7 APPENDIX A: Details of file changes

 In this appendix we examine more closely how files are changed in BASGRA_N compared to BASGRA_2014

7.1 File changes in the top directory

• The file BASGRA.DLL is changed because the new FORTRAN code required re-compilation of the model.

7.2 File changes in subdirectory 'BC'

• This subdirectory contains files that are used to run Bayesian Calibration (BC) of the model and analyse the results.

7.2.1 Changes in BC-files that include a call to 'run model'

• Files that run the model - through a call to the R-function 'run_model' - are changed. This is because running BASGRA_N requires specifying levels of N-fertilisation and N-deposition. So there are small changes in: 'BC_BASGRA_MCMC.R', 'BC_BASGRA_MCMC_init_general.R', and 'BC_plot_outputs_data.R'.

7.2.2 Changes in specification of sites

- It is now possible to include all sites (both for calibration and testing) in the calibration set-up, no need to leave the sites out whose data are not used for calibration. We can now list all the sites in the BC-initialisation file 'BC_BASGRA_MCMC_init_[].R', but we need to specify which of the sites are going to be used in the BC, and which sites are only there for testing and plotting. The idea is to make it a lot easier and quicker to check how model calibration affects BASGRA results for test-sites. In the titles of the plots of output vs. data is stated whether a site was a 'CALIBRATION site' or a 'TEST site'.
- To implement this, changes were made in the definitions of 'calc_logL_s' and 'plot outputs data s' in file BC BASGRA MCMC init general.R.

7.2.3 Changes in specification of measured variables

• Another change is in the specification of the variables whose measurements are used in the calibration. We now no longer need the names of calibration variables in data sets to be identical to BASGRA variable names. If the name of a variable in the data differs from the one used in BASGRA for the same quantity, then we can specify that correspondence in file 'BC_BASGRA_MCMC_init_general.R'.

7.2.4 Changes in files for plotting BC-results

- When many parameters are calibrated (as in the cv-specific BCs with all many parameters), multiple pages are needed to plot results for each parameter. We have now set a maximum of 8 rows and 10 columns per page in the traceplots and prior/posterior histograms.
- We also added new files for plotting BC-results. Three more plots can now easily be made after a BC:
 - Boxplots for all BC-parameters: see 'BC plot parameters boxplots.R'.
 - Plots of total yield (YIELD_TOT) and maximum dry matter (DM_MAX) against cumulative fertilisation (Nfert_TOT): see 'BC_plot_YIELD_TOT&DM_MAX_vs_Nfert_TOT.R'.
 - Plots of selected output variables over time for the prior mode, maximum likelihood and MAP parameter vectors: see function 'BC plot outputs()' defined in the file 'BC plot outputs.R'.

7.2.5 Changes in calculation of the likelihood

- The quantification of data uncertainty (needed for the likelihood function) has changed. In common practice, there are two extreme methods for data uncertainty that we do not want to follow. The two extreme methods are:
 - Assuming that data uncertainty depends on the type of variable (DM, LAI, TILTOT etc.) but not on the value of the variable. So tiny values are assumed to come with the same uncertainty (expressed as the data standard deviation SD) as very large values.
 - Assuming that data uncertainty is proportional to the data value,
 i.e. have a constant coefficient of variation. In this approach the
 SD for small data values becomes very small, making those data
 points extremely influential in the BC.
- Our method lies in between the two extreme methods. Let y be a data value, and let y_max be the highest value for that variable in our whole data set. We specify a coefficient of variation SD_ymax that is appropriate for y_max. So SD_ymax = CV_ymax * y_max. With those definitions our intermediate method of data uncertainty quantification is:

$$- SD_y = CV_y max * sqrt(y_max * y)$$

• That is equivalent to:

$$- SD y = SD ymax * sqrt(y / y max).$$

- This method assigns the highest data uncertainty (SD) to the highest values of y but the SD decreases less than proportionately for smaller y. Instead of scaling linearly with the data value y, the SD now scales with the square root of y.
- We specify (as before) the CV-values in the initialisation file for the BC, which is typically called something like 'BC BASGRA MCMC init...'.

7.3 File changes in subdirectory 'initialisation'

7.3.1 File 'initialise_BASGRA_general.R'

• Declaration of the calendars for N-fertilisation and N-deposition.

- Change in definition of function 'run_model', again to accommodate fertilisation and deposition.
- The vectors "outputNames" and "outputUnits" have been extended with 29 additional output variables, bringing the total (NOUT) to 68.
- The sensitivity analysis function, 'SA()', was changed slightly to allow for different types of plots, to be specified using the new function argument 'type_plot'. The default is still "pdf" but "png" and "jpg" can also be chosen.
- A minor bug in function 'plot outputs Setups' was corrected.

7.3.2 Site-specific initialisation files

• In the initialisation-files for specific sites, e.g. 'initialise_BASGRA_Saerheim_0102_early_Gri.R the N-fertilisation and N-deposition calendars for the site are now specified.

7.4 File changes in subdirectory 'model' (the FORTRAN files)

7.4.1 File 'BASGRA.f90'

- The header of subroutine 'BASGRA' now includes 'CALENDAR_FERT' and 'CALENDAR_NDEP'. The calendar values are stored in arrays named 'DAYS_FERT', 'DAYS_NDEP', 'NFERTV' and 'NDEPV'.
- The parameter array is declared as an array of 120 reals. The number 120 is an upper bound, the actual number of parameters is less than that.
- Additional state variables are declared and their initial values set.
- Additional intermediate and rate variables are declared.
- Five new subroutines are called: 'N_fert', 'N_dep', 'CNsoil', 'Nplant' and 'Digestibility'.
- The call to subroutine 'Growth' now has three extra inputs and one extra output.
- The call to subroutine 'FRDRUNIR' is simplified (variables DRAIN and RUNOFF no longer passed through the header).

- There are many additional output variables.
- There are 8 additional state equations for the new state variables (one plant variable, NSH, and seven soil variables: CLITT, CSOMF, CSOMS, NLITT, NSOMF, NSOMS, NMIN).
- There are calculations that resemble state equations (but are in fact transformations) for deriving total fertilisation (Nfert_TOT) and maximum aboveground dry matter (DM MAX).
- There are additional calculations for a range of different output variables relevant to dry matter distribution, protein content, ash content, cell-wall content and digestibility.

7.4.2 File 'environment.f90'

• This file is not changed.

7.4.3 Parameterisation files

• The file 'set_params.f90' now sets the values for an array of 107 parameters (previously it was 81). The extra parameters are declared in the files 'parameters_plant.f90' and 'parameters_site.f90'.

7.4.4 File 'plant.f90'

- This file has been changed much to include N-processes in plants.
- New variables are being declared.
- Alterations to subroutine 'growth':
 - Subroutine 'growth' has three additional inputs (LAI,NSH,NMIN) and one additional output (NSHmob).
 - The first part of the subroutine, up to and including the first estimates for the "sinks" GLAISI, GLVSI and GSTSI, is unaltered.
 But then nitrogen-processes are invoked to possibly reduce those sink strengths.
 - First, there is a calculation of how much excess N there is in the shoot, i.e. the difference between the amount of N in the shoot (NSH) and the amount expected if N would follow the same decreasing profile as light. If the excess is positive, it is

remobilised at a constant relative rate (time constant parameter TCNSHMOB). The amount of N thus becoming available for growth from within the plants is called 'NSHmob'. Total N available for growth, 'NSOURCE' is then calculated as NSHmob plus a constant fraction of soil mineral N (NMIN divided by time constant TCNUPT).

- The 'shoot sink strength for N', NSINK is calculated as the sum of the first estimates of GLVSI and GSTSI, times the constant maximum NC-ratio of shoot tissue (parameter NCSHMAX).
- Then the growth realisation factor fNgrowth is defined as NSOURCE/NSINK, but not exceeding 1. Finally, the shoot sink strengths are revised by multiplying them with fNgrowth. Allocation then proceeds as before.

• Alterations to subroutine 'Foliage2':

Subroutine 'Foliage2' has a few cosmetic changes (e.g. renaming intermediate variable for potential site filling, TV2, to the clearer name FSPOT) and one major change: the rate of leaf appearance RLEAF is now proportional to the N-growth realisation factor fNgrowth.

• New subroutine 'Nplant'

- The new subroutine Nplant is used to calculate N-fluxes within the plants and between plants and environment.
- First, three intermediate variables are calculated: (1) the normalised amount of N in the shoots (NSHNOR, i.e. the amount of N in shoots divided by the maximum allowable N defined as shoot C multiplied with the maximum shoot N-C ratio NCSH-MAX), (2) the maximum allowable value of the nitrogen extinction coefficient in the vertical sward profile (KNMAX), and (3) the actual value of the nitrogen extinction coefficient (KN). The latter is only approximative, based on application of Taylor-series expansion.
- Then a N-C realisation factor, fNCgrowth, is calculated as a linear function of fNgrowth. The N-C realisation factor is used to reduce the N content of new shoot growth in case of limiting N-availability.

- Then the three processes of changes in shoot N due to growth, senescence and harvesting are calculated, using assumptions about the exponential profile.
- That is followed by calculation of the rates of change in root N due to growth and senescence, assuming a constant N-C ratio in roots.
- Finally, three fluxes are calculated which are the direct consequence of the fluxes calculated above, i.e. they require no additional assumptions or mechanisms. These are: (1) GNmob, the flux from shoot N-remobilisation to new plant growth, (2) NSH-mobsoil, the flux from shoot N-remobilisation to soil in case the NSINK is too small to use up all remobilised nitrogen, (3) Nupt, the rate of N-uptake from the soil.
- New subroutine 'Digestibility'.
 - This subroutine calculates cell-wall contents and digestibilities as a function of phenological stage and aboveground dry matter distribution.
 - Cell-wall fractions in leaves (F_WALL_LV) and stems (F_WALL_ST) increase linearly with phenological stage.
 - The cell-wall fraction of the whole shoot (=leaves + stems + reserves) is the weighted average of the cell-wall contents of the three components (assumed zero for reserves).
 - The cell-wall fraction of total aboveground dry matter (=shoot + stubble) is the weighted average of the cell-wall contents of its components (assumed 100% for stubble).
 - Cell-wall digestibility decreases linearly with phenological stage.
 - Digestibility of leaves, stems, shoot and aboveground dry matter are calculated from their cell-wall content and its digestibility.

7.4.5 File 'resources.f90'

• One new soil variable is calculated, the water-filled pore space (WFPS).

7.4.6 File 'soil.f90'

• This file is one of the three BASGRA FORTRAN-files that has changed the most (together with BASGRA.f90 and plant.f90) to represent C- and N-processes.

- A large number of new variables are declared.
- Altered subroutine 'FRDRUNIR'.
 - This subroutine received one minor change in that DRAIN and RUNOFF are no longer passed through the header of the subroutine but via the list of module-variables at the top of 'soil.f90'.

• New subroutines:

- The new subroutine 'N_fert' checks for each simulation day whether there is a fertilisation event specified in the calendar, and of what magnitude.
- The new subroutine 'N_dep' calculates the N-deposition rate at each simulated day, by linearly interpolating between the values provided in the deposition-calendar.
- The subroutine 'CNsoil' is also new for BASGRA, but it is almost identical to code for forest model BASFOR. This subroutine calculates the transformations of litter and organic matter pools for both C and N, and how much CO2 and mineral N are produced as side- or end-products. The subroutine also calculates N-fixation, N-leaching and N-emission to N2O and NO.

7.5 File changes in subdirectory 'parameters'

• 32 lines were added at the end of 'parameters.txt', one for each new parameter.

7.6 File changes in subdirectory 'data'

We now have data files that include information on variables for nitrogen content, ash-content, cell-wall (fibre) content and digestibility.

8 APPENDIX B: New variables

8.1 Introduction

In this appendix we list all variables that were added when moving from BASGRA to BASGRA_N. We give their names and units. Areas (m2) are always ground area unless otherwise indicated. We distinguish the following types of variables:

1. State variables

2. Non-state variables

- Input variable: Variables whose values are not calculated by the model but defined in the initialization file or imported from an external data file.
- Intermediate variables: Variables that express intermediate results in the calculation of rate or output variables.
- Output variables: Variables whose calculation can be deleted without affecting any of the other model results.
 - Output variables whose identifier is given in quotation marks ("") do not have explicit names in BASGRA.f90, but names are given to them in the plotting routines.
- Rate variables: Variables that directly change state variables. They are part of the state update equation and their unit includes "d-1".
- 3. SOC = Soil Organic Carbon, SOM = Soil Organic Matter, SON = Soil Organic Nitrogen.

8.2 New state variables (BASGRA.f90)

State variable	Unit	Meaning
CLITT	g C m-2	Carbon in litter
CSOMF	g C m- 2	Carbon in fast-decomposing SOM
CSOMS	g C m- 2	Carbon in slow-decomposing SOM
NLITT	g N m- 2	Nitrogen in litter
NSOMF	g N m- 2	Nitrogen in fast-decomposing SOM
NMIN	g N m- 2	Mineral nitrogen
NSOMS	g N m-2	Nitrogen in slow-decomposing SOM
NSH	g N m-2	Nitrogen in shoot

8.3 New non-state variables (BASGRA.f90)

Variable	Unit	Meaning	Type
dCLITT	g C m-2 d-1	Loss of litter C in decomposition	Rate
dCLITTsomf	g C m-2 d-1	Conversion of litter-C to fast SOC	Rate
dCSOMF	g C m-2 d-1	Loss of fast organic C in decomposition	Rate
dCSOMFsoms	g C m-2 d-1	Conversion of fast to slow SOC	Rate
dCSOMS	g C m-2 d-1	Loss of fast organic C in decomposition	Rate
DM	g DM m-2	Dry matter aboveground	Interi
DMLV	g DM m-2	Dry matter leaves	Interi
DMRES	g DM m-2	Dry matter reserves	Interi
DMSH	g DM m-2	Dry matter shoot	Interi
DMST	g DM m-2	Dry matter stems	Interi
DMSTUB	g DM m-2	Dry matter stubble	Interi
DM MAX	g DM m-2	Maximum aboveground dry matter since start of run	Outp
$dNL\overline{I}TT$	g N m-2 d-1	Loss of litter N in decomposition	Rate
DNRT	g N m-2 d-1	Loss of root N in senescence	Rate
DNSH	g N m-2 d-1	Loss of shoot N in senescence	Rate
dNSOMF	g N m-2 d-1	Loss of fast SON in decomposition	Rate
dNSOMS	g N m-2 d-1	Loss of slow SON in decomposition	Rate
F ASH	g m-2	Ash content of shoot dry matter	Outp
F DIGEST DM	-	Digestibility of aboveground dry matter	Outp
F DIGEST DMSH	_	Digestibility of shoot dry matter	Outp
F DIGEST LV	_	Digestibility of leaf dry matter	Outp
F DIGEST ST	_	Digestibility of stem dry matter	Outp
F DIGEST WALL	_	Digestibility of cell walls	Outp
F PROTEIN	g g-1 DM	Crude protein content of shoot dry matter	Outp
F WALL DM	g wall g-1 DM	Fraction of aboveground dry matter that is cell wall	Outp
F WALL DMSH	g wall g-1 DM	Fraction of shoot dry matter that is cell wall	Outp
F WALL LV	g wall g-1 DM	Fraction of leaf dry matter that is cell wall	Outp
F WALL ST	g wall g-1 DM	Fraction of stem dry matter that is cell wall	Outp
GNRT	g N m-2 d-1	Growth of root N	Interi
GNSH	g N m-2 d-1	Growth of shoot N	Rate
HARVNSH	g N m-2 d-1	Harvesting of shoot N	Rate
NCDSH	g N g-1 C	N-C ratio of shoot senescence	Interi
NCGSH	g N g-1 C	N-C ratio of shoot growth	Interi
NCHARVSH	g N g-1 C	N-C ratio of harvested material	Interi
Ndep	g N m-2 d-1	Atmospheric N deposition	Rate
Nemission	g N m-2 d-1 g N m-2 d-1	N emission (NO plus N2O)	Rate
NemissionN2O	g N m-2 d-1 g N m-2 d-1	Emission of nitrous oxide	Outp
NemissionNO	g N m-2 d-1 g N m-2 d-1	Emission of nitrious oxide Emission of nitric oxide	_
Nfert	g N m-2 d-1 g N m-2 d-127	N fertilisation	Outp
	_		Rate
Nfert_TOT Nfixation	g N m-2	Cumulative N-fertilisation from start of run	Outp
	g N m-2 d-1	N fixation	Rate
NILITERATE	g N m-2 d-1	N leaching	Rate
NLITTsomf	g N m-2 d-1	Conversion of litter N to fast SON	Rate
Nmineralisation	g N m-2 d-1	N mineralisation	Rate
NSHmob	g N m-2 d-1	Shoot N Perpolitized shoot N lest to the sail	Rate

8.4 New variables (soil.f90)

Variable	Unit	Meaning	Type
dCLITT	g C m-2 d-1	Loss of litter C in decomposition	Rate
dCLITTrsoil	g C m-2 d-1	Loss of litter C to CO2 in decomposition	${\bf Intermediate}$
$\operatorname{dCLITTsomf}$	g C m-2 d-1	Conversion of litter-C to fast SOC	Rate
dCSOMF	g C m-2 d-1	Loss of fast SOC in decomposition	Rate
dCSOMFrsoil	g C m-2 d-1	Loss of fast SOC to CO2 in decomposition	${\bf Intermediate}$
dCSOMFsoms	g C m-2 d-1	Conversion of fast to slow SOC	Rate
dCSOMS	g C m-2 d-1	Loss of fast SOC in decomposition	Rate
dNLITT	g N m-2 d-1	Loss of litter N in decomposition	Rate
dNSOMF	g N m-2 d-1	Loss of fast SON in decomposition	Rate
dNSOMS	g N m-2 d-1	Loss of slow SON in decomposition	Rate
fN2O	g N g-1 N	Fraction of N emission that is as N2O	${\bf Intermediate}$
fTsoil	-	Temperature effect on decomposition	${\bf Intermediate}$
Ndep	g N m-2 d-1	Atmospheric N deposition	Rate
Nemission	g N m-2 d-1	N emission (NO plus N2O)	Rate
NemissionNO	g N m-2 d-1	Emission of nitric oxide	Output
NemissionN2O	g N m-2 d-1	Emission of nitrous oxide	Output
Nfert	g N m-2 d-1	N fertilisation	Rate
Nfixation	g N m-2 d-1	N fixation	Rate
Nleaching	g N m-2 d-1	N leaching	Rate
NLITTnmin	g N m-2 d-1	Loss of litter N to mineral N	${\bf Intermediate}$
NLITTsomf	g N m-2 d-1	Conversion of litter N to fast SON	Rate
Nmineralisation	g N m-2 d-1	N mineralisation	Rate
NSOMFnmin	g N m-2 d-1	Loss of fast SON to mineral N	${\bf Intermediate}$
NSOMFsoms	g N m-2 d-1	Conversion of fast to slow SON	Rate
rCLITT	g C m-2 d-1	Loss of litter C in run-off	Rate
rCSOMF	g C m-2 d-1	Loss of fast SOC in run-off	Rate
rNLITT	g N m-2 d-1	Loss of litter N in run-off	Rate
rNSOMF	g N m-2 d-1	Loss of fast SON in run-off	Rate
Rsoil	g C m-2 d-1	Soil respiration	Output

8.5 New variables (plant.f90)

Variable	Unit	Meaning
$\overline{\mathrm{DM}}$	g DM m-2	Dry matter aboveground
DMLV	g DM m-2	Dry matter leaves
DMRES	g DM m-2	Dry matter reserves
DMSH	g DM m-2	Dry matter shoot
DMST	g DM m-2	Dry matter stems
DMSTUB	g DM m-2	Dry matter stubble
DNRT	g N m-2 d-1	Loss of root N in senescence
DNSH	g N m-2 d-1	Loss of shoot N in senescence
${ m fNCgrowth}$	-	Effect of N-limitation on N-C ratio of growing tissue
${ m fNgrowth}$	-	Nitrogen source-sink ratio
F_DIGEST_DM	-	Digestibility of aboveground dry matter
F_DIGEST_DMSH	-	Digestibility of shoot dry matter
F_DIGEST_LV	-	Digestibility of leaf dry matter
F_DIGEST_ST	-	Digestibility of stem dry matter
F_DIGEST_WALL	-	Digestibility of cell walls
F_DIGEST_WALL_MIN	-	Minimum digestibility of cell walls
F_WALL_DM	g wall g-1 DM	Fraction of aboveground dry matter that is cell wall
F_WALL_DMSH	g wall g-1 DM	Fraction of shoot dry matter that is cell wall
F_WALL_LV	g wall g-1 DM	Fraction of leaf dry matter that is cell wall
F_WALL_LV_MIN	-	Minimum fraction of leaf dry matter that is cell wall
F_WALL_ST	g wall g-1 DM	Fraction of stem dry matter that is cell wall
F_WALL_ST_MIN	-	Minimum fraction of stem dry matter that is cell wall
GNmob	g N m-2 d-1	Contribution of mobilised N to growth
GNRT	g N m-2 d-1	Growth of root N
GNSH	g N m-2 d-1	Growth of shoot N
HARVNSH	g N m-2 d-1	Harvesting of shoot N
KN	m2 m-2 leaf	Nitrogen extinction coefficient
KNMAX	m2 m-2 leaf	Maximum value of nitrogen extinction coefficient
NCDSH	g N g-1 C	N-C ratio of shoot senescence
NCGSH	g N g-1 C	N-C ratio of shoot growth
NCHARVSH	g N g-1 C	N-C ratio of harvested material
NSH	g N m-2	Nitrogen in shoot
NSHK	g N m-2	Nitrogen in shoot if N-profile equals light-profile
NSHmob	g N m-2 d-1	Shoot N
NSHmobsoil	g N m-2 d-1	Remobilised shoot N lost to the soil
NSHNOR	-	Normalised shoot nitrogen content
Nupt	g N m-2 d-1	N uptake

9 APPENDIX C: New parameters

9.1 Introductory comments

In this appendix we list all parameters that were added when moving from BASGRA to BASGRA_N. We give their names and units. Areas (m2) are always ground area unless otherwise indicated. SOC = Soil Organic Carbon, SOM = Soil Organic Matter.

9.2 New parameters in BASGRA.f90

Parameter	Unit	Meaning	Declared where	Quantified wh
CLITT0	g C m-2	Initial value of CLITT	$parameters_site.f90$	parameters.tx
CNLITT0	g C g-1 N	Initial C-N ratio of litter	$parameters_site.f90$	parameters.tx
CNSOMF0	g C g-1 N	Initial C-N ratio of fast SOM	$parameters_site.f90$	parameters.tx
CNSOMS0	g C g-1 N	Initial C-N ratio of slow SOM	$parameters_site.f90$	parameters.tx
CSOM0	$\rm g~C~m$ -2	Initial value of	$parameters_site.f90$	parameters.tx
FCSOMF0	$\rm g \ C \ g1 \ C$	Initial fraction of SOC that is fast	$parameters_site.f90$	parameters.tx
NCSHMAX	g N g-1 $^{\circ}$	Maximum N-C ratio of shoot	$parameters_plant.f90$	parameters.tx
NMIN0	g N m- 2	Initial value of soil mineral N	$parameters_site.f90$	parameters.tx

9.3 New parameters in soil.f90

Parameter	Unit	Meaning	Declared
FLITTSOMF	g g-1	Fraction of decomposed litter becoming fast SOM	paramete
FSOMFSOMS	g g-1	Fraction of decomposed fast SOM	paramete
KNEMIT	g N g-1 N d-1	Fraction of mineral N emitted in wet soil	paramete
KNFIX	g N g-1 C	Nitrogen fixation per unit of root growth	paramete
RFN2O	-	Sensitivity of N-emission partitioning to soil wetness	paramete
RNLEACH	g N g-1 N	Relative concentration of mineral N in leaching water	paramete
RRUNBULK	g g-1	Relative concentration of soil in run-off water	paramete
TCLITT	d	Time constant of litter decomposition at 10 deg C	paramete
TCSOMF	d	Time constant of fast SOM decomposition at 10 deg C	paramete
TCSOMS	d	Time constant of slow SOM decomposition at 10 deg C	paramete
TMAXF	$\deg C$	Temperature at which decomposition is maximal	paramete
TSIGMAF	$\deg C$	Resilience of decomposition to temperature change	paramete
WFPS50N2O	-	Water filled pore space at which N-emission is half N2O	paramete

9.4 New parameters in plant.f90

Parameter	Unit	Meaning	Declared where
FNCGSHMIN	-	Relative minimum N-C ratio of growing tissue	parameters_plant.f90
NCR	g N g-1 C	N-C ratio of roots	$parameters_plant.f90$
NCSHMAX	g N g-1 C	Maximum N-C ratio of shoot	$parameters_plant.f90$
TCNSHMOB	d	Time constant of shoot N remobilisation	$parameters_plant.f90$
TCNUPT	d	Time constant of soil mineral N uptake	$parameters_plant.f90$

10 APPENDIX D: New constants

10.1 Introductory comments

In this appendix we list all constants that were added when moving from BASGRA to BASGRA_N. We give their names and units. Areas (m2) are always ground area unless otherwise indicated.

10.2 New constants in BASGRA.f90

Constant	Value	Unit	Meaning	Declared where	$\overline{\zeta}$
YIELDI	0.	g DM m-2 d-1	Initial value of yield	$parameters_plant.f90$	р
	6.25	g g-1 N	Protein per unit N	-	В
	0.069	g g-1 DM	Ash content at zero protein content	-	В
	0.14	g g-1 protein	Additional ash content per g protein	_	В

10.3 New constants in soil.f90

Constant	Value	Unit	Meaning	Declared whe
	0.001	m mm-1	Unit conversion	-
	2.	$\rm deg C\text{-}1$	Constant in temperature effect on SOM decomposition	-
	10.	$\deg C$	Constant in temperature effect on SOM decomposition	-

10.4 New constants in plant.f90

Constant	Value	Unit	Meaning	Declared where	Qua
	0.25	-	Constant in calculation of N extinction coefficient	-	plan
	5/8	_	Constant in calculation of N extinction coefficient	-	plan
	2/3	_	Constant in calculation of N extinction coefficient	-	plan
	1.5	-	Constant in calculation of N extinction coefficient	-	plan
	3	-	Constant in calculation of N extinction coefficient	=	plan