

Supplement of

The biogeochemical model Biome-BGCMuSo v6.2 provides plausible and accurate simulations of the carbon cycle in central European beech forests

Katarína Merganičová et al.

Correspondence to: Katarína Merganicová (k.merganicova@forim.sk) ˇ

The copyright of individual parts of the supplement might differ from the article licence.

Table S1 List of abbreviations

Description of simulation steps

Simulations are performed in three steps: (1) spin-up run, (2) transient run, (3) normal run.

Spin-up is a self-initialisation procedure that generates the initial state of the ecosystem using the information about the site, soil, and vegetation type. The spin-up starts from the bare ground with no soil organic matter, a small amount of carbon in leaves, and 50% soil water saturation (which can be set in INI file). During spinup, constant or annually varying regular mortality and fire mortality are allowed, while no management interventions are simulated. A spin-up run lasts several hundred to several thousand years during which carbon stock in an ecosystem is accumulated until a steady state is achieved in soil, when the simulation stops (Thornton and Rosenbloom 2005; Merganičová and Merganič 2014).

A transient run bridges the spin-up and normal runs to avoid the undesired behaviour of simulation outputs due to the sudden changes in CO2 and N-deposition between the two runs (see, for example, (Hidy et al., 2021). During the transient run, constant or annually varying regular natural mortality and fire mortality and management interventions are allowed. It typically lasts several decades, while the length is pre-defined by a user.

A normal run simulates the development of the current target ecosystem (or a future scenario), and it is used to address different research questions, for example, the impact of different climate, N deposition and/or management scenarios on the simulated ecosystem including temporal changes in CO2, and N deposition on growth. Its length, mortality and management settings depend on user´s requirements.

Table S2 Overview of data sources in the database per country and data group. X indicates that data are available for all sites in the specific country, (X) indicates that the data are available for some plots

Figure S1 Dynamic mortality rates applied to simulate natural mortality of regeneration after clearcut (a) based on the compiled information on the survival rates of regeneration from experimental studies focusing on European beech (Hülsmann et al., 2018; Barna et al., 2011) and mortality rates of unmanaged forests (b) simulated using an elliptical function (Merganičová and Merganič, 2014).

Figure S2 Impact of nitrogen fixation Nfix (a) and C:N ratio in leaves (b) on carbon stock in soil, aboveground wood, and litter (SoilC, AbgwC, and LitterC, respectively; all in kgC m⁻²) along the whole tested parameter ranges.

Figure S3 Histograms of C:N ratios in leaves derived from the TRY (Kattge et al., 2020) database (a) and measurements performed at ICP Forests plots in Slovakia (b).

Figure S4 Analysis of trends in variable change with regard to the increasing value of parameters. Blue colour indicates that increasing the parameter value causes an increase in the particular output variable, while the red colour indicates the reduction of the output variable with the increasing parameter value. If both blue and red columns occur above each other for one parameter, the increase of the parameter value resulted in both increasing and decreasing values of the output variable. The trend value gives the proportion of increasing and decreasing values. AbgwC, SoilC, and LitterC stands for carbon stock in aboveground wood, soil, and litter, respectively.

Figure S5 Comparison of observed and simulated time series of carbon stocks in the aboveground wood (AbgwC) using a priori, site-specific (indicated by site identifications), and multi-site (MSMV) optimised sets of ecophysiological parameters for HU1 calibration site. The colours indicate sets of ecophysiological parameters that were used for simulations with BBGCMuSo. The red dashed line represents 1:1 line, when the simulated AbgwC is equal to the observed AbgwC.

Figure S6 Relationships between modelled carbon stock in aboveground wood (AbgwC), soil (SoilC), and litter (LitterC) based on 100,000 Monte Carlo simulations performed for one site during the calibration process. Black dots represent individual simulations, red diamonds represent the best 25 variants selected based on the calculated AbgwC likelihood during GLUE calibration. Note that SoilC and LitterC are represented by mean values over the whole normal run simulations, while AbgwC is represented by the maximum value (hence the value from the last year of simulations), because normal run simulations started with zero AbgwC due to the simulated clearcutting at the beginning. Green triangles represent field observations of respective variables, while SoilC was measured only once, hence this value was taken as a constant to plot all observed AbgwC values. The green rectangular area represents the space defined by field observations of AbgwC and variable ranges of SoilC and LitterC reported in the literature (Pavlenda and Pajtík, 2010).

Figure S7 Relationships between mean differences of carbon stock in aboveground wood (AbgwC) and soil (SoilC) calculated as arithmetic means of the modelled value minus the observed value of the respective variable in the particular years. The modelled data come from site-specific Monte Carlo simulations used for model calibration. Colours represent individual sites, for which the observed values of both AbgwC and SoilC were available. Red lines indicate zero differences between modelled and observed values.

- AbgwC - SoilC - LitterC - KombinedC - SumC

Figure S8 Robustness test of calibrated site-specific and multi-optimised parameter values based on decision tree analysis. Black dots are site-specific optimised parameter values, vertical red and blue lines represent the a priori and the multi-site optimised values, respectively. Background transparent coloured horizontal lines represent the tested parameter range, while non-transparent coloured lines show the optimised parameter ranges based on decision trees performed for carbon stock in aboveground wood (purple), soil (blue), and litter (green). The khaki interval is an optimised parameter range derived as an intersection of the three ranges for individual variables defined above. The red interval in an optimised parameter range derived for the sum of the three carbon stocks. If the optimised ranges for individual variables or sites did not overlap, the final range was derived based on the prevailing intersections.

Figure S9 Spearman correlations of site-specific optimised parameter values to soil characteristics. The colour and the size of the circles indicate the value of the correlation coefficient. Abbreviations of parameters and environmental characteristics are in [Table S1.](#page-1-0)

Figure S10 Relationship between site-specific optimised values of nitrogen fixation (Nfix) and fraction of leaf nitrogen in Rubisco (FLNR)

Figure S11 Linear regressions between site-specific optimised values (SSMV) of canopy light extinction coefficient (CLEC) and carbon stock in the aboveground wood at the standardised age of 63 years (AbgwC) and elevation of 11 calibration sites.

Figure S12 Validation of multi-sites multivariate optimised parameter set based on the simulations of 8 research sites. The figures represent boxplots of the differences between the modelled and observed aboveground wood carbon stock (AbgwC, a), and modelled carbon stock in soil (SoilC, b) and litter (LitterC, c) compared to ranges observed in the field (horizontal red lines represent median (solid line) and 5 and 95% percentiles (dashed lines)). The ranges for carbon stock in soil and litter were taken from (Pavlenda and Pajtík, 2010). The thick horizontal lines of boxplots represent medians, boxes represent the interquartile ranges (IQR), and the vertical lines represent ± 1.5 IQR.

Figure S13 Plausibility of carbon simulated content in aboveground wood, soil and litter (AbgwC, SoilC, LitterC) at the end of spinup simulations performed for all sites in comparison to ranges derived from the literature (horizontal red lines represent median (solid line) and 5 and 95% percentiles (dashed lines)). The ranges for carbon stock in the aboveground wood were taken from (Barna et al., 2011) for over-aged beech forests at average-quality sites. The ranges for carbon stock in soil and litter were taken from (Pavlenda and Pajtík, 2010).

Figure S14 Responses of modelled carbon stock in the aboveground wood (AbgwC) at the standardised stand age of 35 years (left), soil (middle) and litter (right) carbon stocks to sand content in soil (top) and soil texture (bottom). The simulations with BBGCMuSo were conducted for 87 sites distributed across central Europe (see Figure 1).

Figure S15 Multiple linear regressions explaining the variation in site-specific canopy light extinction coefficient (CLEC) values using different combinations of environmental characteristics. The size of the model represents the number of predictors included in the multiple regression model. The figure on the left presents the selected combinations of environmental characteristics, while black squares indicates, which characteristics are included in multiple regression models and black dots indicate their absence in the model. The right figure shows statistical characteristics of derived models as follows: R2—R-squared, R2adj—adjusted R-squared, AIC—AKAIKE information criterion, BIC—Bayesian information criterion, Cp—Mallows' statistic, Sigma—residual standard deviation. The abbreviations of environmental characteristics are explained in [Table S1.](#page-1-0)

Figure S16 Plausibility percentages of BBGCMuSo simulations per calibration site and carbon stock in aboveground wood, soil, litter and all output variables at the same time (AbgwC, SoilC, LitterC, All).

Figure S17 Spearman correlations between selected carbon-related output variables and site characteristics. The colour and the size of the circles indicate the value of the correlation coefficient, and the stars indicate the significance of the correlation (1 star, 2 stars and 3 stars represent 95%, 99% and 99.9% significance levels, respectively). The abbreviations are explained in [Table S1.](#page-1-0)

Figure S18 Spearman correlations between selected carbon-related output variables and soil particle proportions in individual soil layers. The colour and the size of the circles indicate the value of the correlation coefficient, and the stars indicate the significance of the correlation (1 star, 2 stars and 3 stars refer to 95%, 99% and 99.9% significance levels, respectively). The abbreviations are explained i[n Table](#page-1-0) [S1.](#page-1-0) Values behind soil particle groups indicate individual soil layers, while Aver refers to the mean value calculated from all layers.

Figure S19 Relationships between selected output variables and environmental characteristics derived from the BBGCMuSo simulated output of 87 sites distributed across central Europe (see Figure 1).

Figure S20 Relationships between the simulated volumetric soil water content and soil texture based on the BBGCMuSo simulated output of 87 sites distributed across central Europe (see Figure 1).

R code for the model calibration

Here we present excerpts from the R source code that was used in the study to perform the calibration of ecophysiological parameters in BBGCMuSo for European beech (*Fagus sylvatica* $L.$).

library(RBBGCMuso) **#WS2 Sensitivity analysis -- -----------** # For more information visit https://nimbus.elte.hu/agromo/files/musoSensi_usage.html parameters <- read.csv("parameters.csv")

musoSensi (parameters=parameters, iterations = 100000 , varIndex = 2, monteCarloFile = "preservedEpc.csv", skipSpinup = FALSE)

#WS4a Site- and variable-specific generalised likelihood uncertainty (GLUE) optimisation of parameter values--- -----------------------

For more information visit https://github.com/hollorol/RBBGCMuso?tab=readme-ov-file

md <- data.table::fread("LDaboveC_w _OBSERVED.txt")

parameters <- read.csv("parameters.csv")

mylikelihood = list(stemC = (function(x, y){exp(-sqrt(mean((x-y)^2))) }))

calibrateMuso (measuredData = md,

 $dataVar = c(LDaboveC \t w = 3158)$, iterations = 100000,

likelihood = mylikelihood, method="GLUE", skipSpinup=FALSE)

#WS4b Site-specific multivariate identification of plausible simulations based on output constraints-- ----------------------------

PlausibleSim<-subset(Data, LDaboveC_w<70 & SoilC>5 & SoilC<25 & LitterC>0.1 & LitterC<4)

FeasibleRangeCLEC< c(min(PlausibleSim\$CLEC,na.rm=TRUE),max(PlausibleSim\$CLEC,na.rm=TRUE))

…

#WS4c Site-specific multivariate parameter optimisation-- --------- Data\$DifSoilC<-(Data\$SoilC-Data\$SoilCReal) Data\$DifStemC<-(Data\$LDaboveC_w-Data\$stemCReal) Data\$DifLitterC<-(Data\$LitterC-Data\$LitterCReal)

ddply(Data, c("Site","Procesor","IDCal"), summarise, NDifStemC=sum(!is.na(DifStemC)), MinDifStemC=min(DifStemC,na.rm=TRUE), MaxDifStemC=max(DifStemC,na.rm=TRUE), AMDifStemC=mean(DifStemC,na.rm=TRUE), RMSEDifStemC=sqrt(sum((DifStemC)^2 , na.rm = TRUE) / NDifStemC), MSEDifStemC=sum((DifStemC)^2 , na.rm = TRUE) / NDifStemC, MAEDifStemC=sum(abs(DifStemC) , na.rm = TRUE) / NDifStemC, MPEDifStemC=100*sum((DifStemC/stemC) , na.rm = TRUE) / NDifStemC, LikeDifStemC=exp(-RMSEDifStemC), MinModelStemC=min(LDaboveC_w,na.rm=TRUE), MaxModelStemC=max(LDaboveC_w,na.rm=TRUE), AMModelStemC=mean(LDaboveC_w,na.rm=TRUE)

….)

LikeDifSum<-LikeDifLDaboveC_w +LikeDifSoilC+LikeDifLitterC

```
if (LikeDifSum==min(LikeDifSum)) 
{
SSMV_CLEC<-CLEC
…
}
SSMV<-c(SSMV_CLEC, SSMV_FLNR, SSMV_ MSC, SSMV_Nfix, SSMV_VPDC, SSMV_Sseff)
```
#WS4d Multi-site and multivariate parameter optimisation--- ---------

minCLEC<- max(FeasibleRangeCLEC\$minCLEC, na.rm=TRUE)

maxCLEC<- min(FeasibleRangeCLEC\$maxCLEC, na.rm=TRUE) FeasibleRangeCLEC_MS<-c(minCLEC, maxCLEC)

```
…
```
Categorisation<-function(Val,MinVal,MaxVal,NoCategories)

{

VarRange<-MaxVal-MinVal

IntervalWidth<-VarRange/NoCategories

MidInterval<-IntervalWidth/2

VectorCategory<-data.frame(1:NoCategories)

VectorCategory\$Mid<- VectorCategory \$X1.NoCategories*IntervalWidth+MinVal-MidInterval

```
VectorCategory$Dif<-abs(VectorCategory$Mid-Val)
```

```
VectorCategory <- VectorCategory [order(VectorCategory$Dif),]
```

```
Categ<- VectorCategory$X1.NoCategories[1]
```

```
}
```

```
NoCat<-5
DataCat<-c()
for (i in 1:nrow(DataStat))
{
DataCat<-c()
DataCat$Site<-DataStat$Site[i]
DataCat$CLEC_Cat<-Categorisation(DataStat$CLEC[i],MinCLEC,MaxCLEC,NoCat)
…
DataCat$CatJoint<-paste0(DataCat$CLEC_Cat,"_",DataCat$FLNR_Cat,"_",DataCat$MSC_Cat,"_",
               DataCat$Nfix_Cat,"_",DataCat$VPDC_Cat,"_",DataCat$Sseff_Cat)
  }
```
Tab1<-ddply(DataJoint, c("CatJoint"), summarise,

NoVariants<-length(IDCal),

NoSites<-length(unique(Site)),

```
 AMCLEC<-mean(CLEC),
```
..)

MSMV_CLEC<-subset(DataJoint\$AMCLEC, NoSites==max(Tab1\$NoSites))

…

MSMV<-c (MSMV_CLEC, MSMV_FLNR, MSMV_ MSC, MSMV_Nfix, MSMV_VPDC, MSMV_Sseff)

References

Barna, M., Kulfan, J., and Bublinec, E.: Beech and Beech Ecosystems of Slovakia / Buk a bukové ekosystémy Slovenska, Veda, Bratislava, 636 pp., 2011.

Hidy, D., Barcza, Z., Hollós, R., Thornton, P. E., Running, S. W., and Fodor, N.: User's Guide for Biome-BGCMuSo 6.2, 2021.

Hülsmann, L., Bugmann, H., Meyer, P., and Brang, P.: Natürliche Baummortalität in Mitteleuropa: Mortalitätsraten und -muster im Vergleich, Schweiz. Z. Forstwes., 169, 166–174, https://doi.org/10.3188/szf.2018.0166, 2018.

Kattge, J., Bönisch, G., Díaz, S., Lavorel, S., Prentice, I. C., Leadley, P., Tautenhahn, S., Werner, G. D. A., Aakala, T., Abedi, M., Acosta, A. T. R., Adamidis, G. C., Adamson, K., Aiba, M., Albert, C. H., Alcántara, J. M., Alcázar C, C., Aleixo, I., Ali, H., Amiaud, B., Ammer, C., Amoroso, M. M., Anand, M., Anderson, C., Anten, N., Antos, J., Apgaua, D. M. G., Ashman, T.-L., Asmara, D. H., Asner, G. P., Aspinwall, M., Atkin, O., Aubin, I., Baastrup-Spohr, L., Bahalkeh, K., Bahn, M., Baker, T., Baker, W. J., Bakker, J. P., Baldocchi, D., Baltzer, J., Banerjee, A., Baranger, A., Barlow, J., Barneche, D. R., Baruch, Z., Bastianelli, D., Battles, J., Bauerle, W., Bauters, M., Bazzato, E., Beckmann, M., Beeckman, H., Beierkuhnlein, C., Bekker, R., Belfry, G., Belluau, M., Beloiu, M., Benavides, R., Benomar, L., Berdugo-Lattke, M. L., Berenguer, E., Bergamin, R., Bergmann, J., Bergmann Carlucci, M., Berner, L., Bernhardt-Römermann, M., Bigler, C., Bjorkman, A. D., Blackman, C., Blanco, C., Blonder, B., Blumenthal, D., Bocanegra-González, K. T., Boeckx, P., Bohlman, S., Böhning-Gaese, K., Boisvert-Marsh, L., Bond, W., Bond-Lamberty, B., Boom, A., Boonman, C. C. F., Bordin, K., Boughton, E. H., Boukili, V., Bowman, D. M. J. S., Bravo, S., Brendel, M. R., Broadley, M. R., Brown, K. A., Bruelheide, H., Brumnich, F., Bruun, H. H., Bruy, D., Buchanan, S. W., Bucher, S. F., Buchmann, N., Buitenwerf, R., Bunker, D. E., et al.: TRY plant trait database – enhanced coverage and open access, Glob. Change Biol., 26, 119–188, https://doi.org/10.1111/gcb.14904, 2020.

Merganičová, K. and Merganič, J.: The Effect of Dynamic Mortality Incorporated in BIOME-BGC on Modelling the Development of Natural Forests, J. Environ. Inform., 24, 24–31, 2014.

Pavlenda, P. and Pajtík, J.: Monitoring lesov Slovenska, LVÚ Zvolen, Zvolen, NLC, 2010.

Thornton, P. E. and Rosenbloom, N. A.: Ecosystem model spin-up: estimating steady state conditions in a coupled terrestrial carbon and nitrogen cycle model, Ecol. Model., 189, 25–48, https://doi.org/10.1016/j.ecolmodel.2005.04.008, 2005.