

SUPPLEMENTARY MATERIAL

Soil related developments of the Biome-BGCMuSo terrestrial ecosystem model by integrating crop model components

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Abbreviations

SAT: saturation

FC: field capacity

WP: wilting point

HW: hygroscopic water

i : index denoting soil layers (from 1 to 10)

dz^i : thickness of the i^{th} soil layer in cm

SWC^i : actual volumetric water content of the i^{th} soil layer in $\text{m}^3 \text{m}^{-3}$

SWC_{SAT}^i : volumetric water content at saturation of the i^{th} soil layer in $\text{m}^3 \text{m}^{-3}$

SWC_{FC}^i : volumetric water content at field capacity of the i^{th} soil layer in $\text{m}^3 \text{m}^{-3}$

SWC_{WP}^i : volumetric water content at wilting point in the i^{th} soil layer in $\text{m}^3 \text{m}^{-3}$

mid^i : depth of the midpoint of the i^{th} soil layer in m

K_{SAT}^i : saturated hydraulic conductivity of the i^{th} soil layer in cm day^{-1}

1. Runoff

Calculation of *RUNOFF* [$\text{kg H}_2\text{O m}^{-2} \text{ day}^{-1}$] is based on a semi-empirical method that uses the precipitation amount (*PRCP*), the dimensionless runoff curve number (*RCN*), and the actual moisture content status of the topsoil (Williams, 1991). If *PRCP* is less than a critical value (product of a soil type and a moisture content dependent factor; k_{type} and k_{moist}), runoff is equal to zero. Otherwise:

$$RUNOFF = \frac{(PRCP - k_{moist} \cdot k_{type})^2}{prcp + (1 - k_{moist}) \cdot k_{type}}, \text{ if } PRCP > k_{moist} \cdot k_{type}$$

$$k_{type} = 254 \cdot \frac{100}{RCN} - 1$$

$$k_{moist} = 0.15 \cdot \frac{SWC_{SAT}^1 - SWC^1}{SWC_{SAT}^1 - SWC_{HW}^1}$$

where: SWC_{SAT}^1 , SWC_{HW}^1 and SWC^1 are the saturated, the hygroscopic and the actual volumetric water content of the top soil layer.

The amount of runoff is affected also by the setting of pond water calculation: first the pond water accumulation is calculated (see details in Section 3.1), only the surplus above the maximum pond depth leaves as runoff.

2. Downward (gravitational) water flow

The percolation calculations (tipping bucket method) are carried out layer by layer starting from the 1st soil layer down to the 9th soil layer. The bottom (10th) soil layer is special: the percolating water (and dissolved materials) from the bottom layer is a net loss from the system. It is assumed that the soil can hold moisture against gravity up to its field capacity. One of the most important variables of percolation calculation is the drainage coefficient (*DC*) which determines the amount of water leaving a layer in a day. *DC* is a soil input parameter but in case it is not provided by the user, it is estimated from the hydraulic conductivity:

$$DC^i = 0.1122 \cdot K_{SAT}^i{}^{0.339}$$

Percolation calculation is different on rainy and rainless days, but in both cases uses daily time step. On rainy days, if the inflowing water amount ($INFILT^i$; *cm*) is greater than the water holding capacity ($HOLD^i$, *cm*) of the given layer, the drainage water that leaves the layer (DRN^i , *cm*) is calculated as follows:

- $HOLD^i = (SWC_{SAT}^i - SWC^i) \cdot dz^i$
- drainage from the water content stored in the layer [*cm*]:

$$DRAIN^i = DC \cdot (SWC_{SAT}^i - SWC_{FC}^i) \cdot dz^i$$

- total drainage from and through a soil layer [cm]:

$$DRN^i = INFILT^i - HOLD^i + DRAIN^i$$

- total drainage is limited by saturated conductivity: if $DRN^i \geq K_{SAT}^i$:

$$(DRN^i)_{limited} = K_{SAT}^i$$

- water content is updated: $SWC^i = SWC^i + \frac{INFILT^i - (DRN^i)_{limited}}{dz^i}$
- the excess water ($EXCESS^i$; cm) is redistributed in layers above (from the actual layer up to the 1st one): $EXCESS^i = DRN^i - K_{SAT}^i$
- first the capacity of the layer above is filled and in the case of remaining excess moving one layer above
- if at the end of the redistribution (in the top soil layer) $EXCESS^i$ is greater than 0, its value is added to pond water and/or runoff depending on the actual pond depth and maximal pond depth, which is an input soil parameter
- infiltration into the next layer is the drainage from the layer above:

$$INFILT^{i+1} = DRN^i$$

If $INFILT^i$ is less than or equal to $HOLD^i$:

- water content update: $SWC^i = SWC^i + INFILT^i/dz^i$
- drainage is calculated only if soil moisture content is above field capacity, otherwise it is zero:

$$DRN_i = DC \cdot (SWC^i - SWC_{FC}^i) \cdot dz^i$$

- drainage is limited by the saturated conductivity: $DRN^i \leq K_{SAT}^i$
- state update moisture content with drainage: $SWC^i = SWC^i - DRN^i/dz^i$
- infiltration into the next layer is the drainage of the above one: $INFILT^{i+1} = DRN^i$

On rainless days the calculation is simpler: there is no infiltration at the top of the soil profile

- Maximum of drainage ($DRMX$; cm) is greater than zero only if soil moisture content is above field capacity

$$DRMX^i = DC \cdot (SWC^i - SWC_{FC}^i) \cdot dz^i$$

- $HOLD$ is greater than zero only if soil moisture content is below field capacity

$$HOLD^i = (SWC_{FC}^i - SWC^i) \cdot dz^i$$

- Drainage rate in the top layer: $DRN^1 = DRMX^1$

- Drainage rate in layers below: $DRN^i = DRN^{i-1} + DRM^i - HOLD^i$
- Drainage is limited by saturated conductivity: $DRN^i \leq K_{SAT}^i$
- The SWC is updated from 9th layer to 2nd layer with saturation as the upper limit:

$$SWC^i = SWC^i + (DRN^{i-1} - DRN^i)/dz^i$$

$$\text{if } SWC^i > SWC_{SAT}^i$$

$$DRN^{i-1} = (SWC_{SAT}^i - SWC^i) \cdot dz^i + DRN^i$$

$$SWC^i = SWC_{SAT}^i$$

- Status update of SWC in the top (1st) layer: $SWC^1 = SWC^1 - DRN^1/dz^1$

3. Capillary water flow

The diffusion calculations follow the formulae of the 4M model (Fodor et al., 2014). The downward diffused water from the bottom active (9th) layer is a net loss for the soil system, while the upward diffusion flux from the passive (10th) layer is a net gain.

- water flow between the actual layer and the one below is estimated with the product of the gradient ($GRAD$) of the normalized water contents ($THET$) between two adjacent layers and the diffusivity at the border of the two layers ($DBAR$). Diffusivity is also assumed to be a function of the normalized water contents of the two adjacent layers.

$$ESW^i = SWC_{FC}^i - SWC_{WP}^i$$

$$ESW^{i+1} = SWC_{FC}^{i+1} - SWC_{WP}^{i+1}$$

$$THET^i = \min(SWC_{act}^i - SWC_{WP}^i; ESW^i)$$

$$THET^{i+1} = \min(SWC_{act}^{i+1} - SWC_{WP}^{i+1}; ESW^{i+1})$$

weighted average water content of the two layers:

$$inner_{THET} = \frac{THET^i \cdot dz^i + THET^{i+1} \cdot dz^{i+1}}{dz^i + dz^{i+1}}$$

$$DBAR = \min(p1_{diffus} * \exp(p2_{diffus} * inner_{THET}), p3_{diffus})$$

$$inner_{ESW} = \frac{ESW^i \cdot dz^i + ESW^{i+1} \cdot dz^{i+1}}{dz^i + dz^{i+1}}$$

where $p1_{diffus}$, $p2_{diffus}$, $p3_{diffus}$ are the parameters of diffusion calculation, default values are 0.88, 35.4 and 100, respectively.

- gradient between the actual and the layer below:

$$GRAD = inner_{ESW} \cdot \left(\frac{THET^{i+1}}{ESW^{i+1}} - \frac{THET^i}{ESW^i} \right)$$

- water flow between the actual and the layer below:

$$FLOW = \frac{DBAR * GRAD}{dz^i + dz^{i+1}} \cdot 0.5$$

4. Soil evaporation

The method calculates the cumulated soil evaporation (*soilEvap*) in two phases (Ritchie, 1972). In the first phase, if the cumulated evaporation is less than a critical value (*soilEvapLIM* [mm]: soil input parameter), and hence the evaporation is not limited. In the second phase, if the cumulated evaporation is greater than *soilEvapLIM*, soil evaporation is reduced. Variables *soilEvapCUM1* and *soilEvapCUM2* are the cumulated soil evaporation values in the first and the second evaporation phase, respectively. Potential infiltration (*infiltrPOT* [mm]) is the water from precipitation or melting snow, or pond water, which can decrease the cumulated soil evaporation values. Depending on the *infiltrPOT* amount, *soilEvapCUM2* is decreased first till it becomes zero, than *soilEvapCUM1* is reduced. Potential soil evaporation (*soilEvapPOT* [mm]) is calculated based on the Penman-Monteith method in daily time scale (see Section 3.3).

In the second evaporation phase the cumulative evaporation is a quadratic function of the time (number of days) since the last rainfall event (*dSr*).

First evaporation phase: $soilEvapCUM1 < soilEvapLIM$

$$dSr = 0$$

$$soilEvapCUM1 = 0; \text{ if } infiltrPOT \geq soilEvapCUM1$$

$$soilEvapCUM1 = soilEvapCUM1 - infiltrPOT; \text{ if } infiltrPOT < soilEvapCUM1$$

$$soilEvapCUM1 = soilEvapCUM1 + soilEvapPOT$$

if $soilEvapCUM1 > soilEvapLIM$:

$$soilEvap = soilEvapPOT - 0.4 \cdot (soilEvapCUM1 - soilEvapLIM)$$

$$soilEvapCUM2 = 0.6 \cdot (soilEvapCUM1 - soilEvapLIM)$$

$$dSr = \left(\frac{soilEvapCUM2}{3.5} \right)^2$$

$soilEvapCUM1 = soilEvapLIM$ if $soilEvapCUM1 \leq soilEvapLIM$:

$$soilEvap = soilEvapPOT$$

Second evaporation phase: $soilEvapCUM1 \geq soilEvapLIM$

If $infiltrPOT \geq soilEvapCUM2$:

$$dsr = 0$$

$$infiltrPOT = infiltrPOT - soilEvapCUM2$$

$$soilEvapCUM2 = 0$$

$$soilEvapCUM1 = 0 ; \text{if } infiltrPOT \geq soilEvapLIM$$

$$soilEvapCUM1 = soilEvapCUM1 - infiltrPOT; \text{if } infiltrPOT < soilEvapLIM$$

$$soilEvapCUM1 = soilEvapCUM1 + soilEvapPOT$$

if $soilEvapCUM1 \leq soilEvapLIM$:

$$soilEvap = soilEvapPOT - 0.4 \cdot (soilEvapCUM1 - soilEvapLIM)$$

$$soilEvapCUM2 = 0.6 \cdot (soilEvapCUM1 - soilEvapLIM)$$

$$dsr = \left(\frac{soilEvapCUM2}{3.5} \right)^2$$

if $soilEvapCUM1 > soilEvapLIM$:

$$soilEvap = soilEvapPOT$$

If $infiltrPOT < soilEvapCUM2$:

$$soilEvapCUM2 = soilEvapCUM2 - infiltrPOT$$

$$dsr = \left(\frac{soilEvapCUM2}{3.5} \right)^2$$

$$dsr = dsr + 1$$

$$soilEvap = 3.5 \cdot dsr^{0.5} - soilEvapCUM2$$

limitation: potential evaporation: $soilEvap \leq soilEvapPOT$

Soil evaporation cannot be larger than the available soil water content ($soilwAVAIL$) in the top layer which is the difference between the actual and the hygroscopic water content. The hygroscopic water content is a soil input parameter.

$$soilEvap = \min(soilEvap, soilwAVAIL)$$

$$soilEvapCUM2 = soilEvapCUM2 + soilEvap$$

$$dsr = \left(\frac{soilEvapCUM2}{3.5} \right)^2$$

5. Transpiration

Transpiration demand (TD) is distributed across the soil layers according to the root distribution. From the plant specific root parameters and the actual root weight Biome-BGCMuSo calculates the actual rooting depth (RL), the number of the layers where roots can be found together with the root mass distribution across the layers. If there is no enough water in the given soil layer to provide the transpiration demand, the transpiration flux from the actual layer (T^i) is limited, and below WP T^i is equal to zero. The sum of T_i values across the root zone gives the actual transpiration flux (T).

$$TD^i = TD \cdot rootprop^i$$

$$rootprop^i = RDP \cdot \frac{dz^i}{RL} \cdot e^{-RDP \cdot \frac{mid^i}{RL}}$$

$$T^i = TD^i \quad \text{if } SWC^i \geq SWC_{WP}^i \text{ and } TD^i \leq SWC^i - SWC_{WP}^i$$

$$T^i = SWC^i - SWC_{WP}^i \quad \text{if } SWC^i \geq SWC_{WP}^i \text{ and } TD^i > SWC^i - SWC_{WP}^i$$

$$T^i = 0 \quad \text{if } SWC^i < SWC_{WP}^i$$

where: $rootprop^i$ is the proportion of the root length in the given soil layer, RDP is the rooting distribution plant input parameter (detailed description in User's Guide).

6. FC-rising effect of groundwater

The FC-rising effect of groundwater ($GWeff$) for the layers above the water table (WT) is calculated based on the ratio of actual ($GWdist$) and critical distance (CF_{act}) from WT, but only after the layers below have already been charged up to their modified FC values. $GWeff$ is equal to zero for layers above the capillary fringe.

$$GWeff = 1 - \frac{GWdist}{CF_{act}} \quad ; \text{if } CF_{act} > GWdist > 0$$

The modified FC due to the close groundwater table is calculated with a linear function:

$$SWC_{FCmod} = SWC_{FC} + GWeff \cdot (SWC_{SAT} - SWC_{FC})$$

The water flux coming from the groundwater on a given day and in a given layer ($dischargeGW$; $\text{kgH}_2\text{O m}^{-2} \text{day}^{-1}$) is a net gain for the soil profile above the water table and is the function of drainage coefficient (DC) of the given layer.

$$dischargeGW = (SWC_{FCmod}^i - SWC^i) \cdot dz^i \cdot \rho_{water} \cdot DC \quad \text{if } SWC_{FCmod}^i > SWC^i$$

$$dischargeGW = 0 \quad \text{if } SWC_{FCmod}^i \leq SWC^i$$

7. Nitrogen mineralization function

The nitrogen mineralization fluxes of the litter pools are the function of the corresponding potential litter loss rate ($potCloss$ in $\text{kg C m}^{-2} \text{ day}^{-1}$), C:N ratio (kg C kg N^{-1}) and respiration fraction. The nitrogen mineralization fluxes of the SOM pools are the function of carbon loss rate, which is the function of potential rate constant (k_base : reciprocal of residence time in day^{-1}), and environmental integrated response function (F_r).

$$potM_{AB}^i = \frac{potCloss_A^i \cdot (1 - rf_A - CN_B^i / CN_A^i)}{CN_B^i}$$

$$potCloss_A^i = k_A^i \cdot CN_B^i$$

$$k_A^i = k_base_A \cdot F_r$$

where: $potCloss_A^i$ is the potential carbon loss of the source pool (A) in the actual layer, rf_A is the respiration factor of the source pool, CN_A^i and CN_B^i are the C:N ratios of the given source and target compartments in the actual layer, respectively; k_A^i is the actual rate constant scalar of the source pool in the i^{th} layer, k_base_A is the potential rate constant scalar of the source compartment (soil input parameter, see detailed in User's Guide), F_r is the response function of the i^{th} layer. A index denotes the source pools (L1, L2, L4, S1, S2, S3), B index denotes the target pools (S1, S2, S3, S4), AB index denotes the transformations between different pools: L1-S1, L2-S2, L4-S3, S1-S2, S2-S3 and S3-S4 (see Figure 4 in Section 4.2).

The decomposition of the passive SOM pool (S4) is special: only mineralization is assumed, and the respiration factor is supposed to be equal to 1, namely all released carbon is respired, no target pool is defined.

$$potM_{S4}^i = \frac{potCloss_{S4A}^i}{CN_B^i}$$

The response function (F_r) of the transformation processes is the product of depth, water and temperature dependent factors ($Fr(d)_D^i$, $Fr(SWC)_D^i$, and $Fr(T)_D^i$, respectively) calculated layer by layer.

The $Fr(d)_D^i$ factor of the i^{th} layer is the exponential function of ratio the layer's midpoint (mid_i in m) and *e-folding depth of decomposition rate's depth scalar* (ED in m; see detailed in the User's Guide):

$$F_r(d)_D^i = e^{-\frac{mid^i}{ED}}$$

The $Fr(SWC)_D^i$ factor is zero below HW, is equal to 1 between FC and a critical SWC (SWC_{crit2}^i) is defined by a soil input parameter (see User Guide).

$$F_r(SWC)_D^i = \frac{SWC_{act}^i - SWC_{HW}^i}{SWC_{FC}^i - SWC_{HW}^i}; \quad \text{if } SWC_{HW}^i < SWC_{act}^i < SWC_{FC}^i$$

$$F_r(SWC)_D^i = \frac{SWC_{SAT}^i - SWC_{act}^i}{SWC_{SAT}^i - SWC_{crit2}^i}; \quad \text{if } SWC_{crit2}^i < SWC_{act}^i < SWC_{SAT}^i$$

The $F_r(T)_D^i$, is the bell function of the soil temperature in the given layer (T_{soil}^i):

$$F_r(T)_D^i = \frac{Tp1_{decomp}}{1 + \left(ABS \left(\frac{T_{soil}^i - Tp4_{decomp}}{Tp2_{decomp}} \right) \right)^{Tp3_{decomp}}}$$

8. Nitrification

The first step of nitrification calculation is to determine the net ammonia mineralization flux in the actual layer (MI_{netNH4}^i). Net ammonia mineralization is the sum of mineralization fluxes MI^i (detailed in Section 4.2) and the ammonia mineralization of the passive humus pool ($potM_{s4}^i$).

Nitrification flux is calculated layer by layer based on the following Equation:

$$NI^i = MI_{netNH4}^i \cdot NI_{netMI} \cdot F_r(Ts)_{NI}^i \cdot F_r(SWC)_{NI}^i \cdot F_r(pH)_{NI}^i$$

where: NI_{netMI} is the *net mineralization proportion of nitrification parameter* soil input parameter, $F_r(Ts)_{NI}^i$, $F_r(SWC)_{NI}^i$, $F_r(pH)_{NI}^i$ are the response functions of soil temperature, soil water content and pH in the actual layer, respectively. $F_r(Ts)_{NI}^i$, is the same as $F_r(Ts)_D^i$, $F_r(SWC)_{NI}^i$ is also a trapezoidal function (such as $F_r(SWC)_D^i$) depending on soil input parameter (detailed in the User Guide). $F_r(pH)_{NI}^i$ is an empirical, exponential function of pH (Parton et al., 2001). If the value of the response function is zero (below a critical value of the given soil properties), the nitrification process is totally limited. If the value of the response function is 1 (above a critical value of the given soil properties), the process is not limited. In case the actual soil water content exceeds the optimal soil water content, the response function can decrease accounting for the saturation related stress (anoxic soil).

9. N₂O-emission and N-emission

During both nitrification and denitrification N₂O-emission occurs which (added to the N₂O-flux originated from grazing processes) contributes to the total N₂O-emission of the simulated ecosystem.

In Biome-BGCMuSo v6.2 a fixed part (set by the coefficient of N₂O emission of nitrification soil input parameter; User Guide) of nitrification flux is lost as N₂O and not converted to NO₃.

During denitrification, nitrate transforms to N₂ and N₂O gas depending on the environmental conditions: NO₃ availability, total soil respiration (proxy for microbial activity), soil water content and pH. The following equation is used to calculate the ratio of N₂ and N₂O that is generated during denitrification:

$$R_{N_2:N_2O} = \min[F_r(NO_3)_{DN}^i \cdot F_r(CO_2)_{DN}^i] \cdot F_r(SWC)_{DN}^i \cdot F_r(pH)_{DN}^i$$

where $R_{N_2:N_2O}$ is the ratio of N₂ and N₂O gas (both expressed as N equivalent mass), $F_r(NO_3)_{DN}^i$ represents the effect of NO₃ availability, $F_r(CO_2)_{DN}^i$ is a total soil respiration related modifying factor (proxy for microbial activity), $F_r(SWC)_{DN}^i$ represents the effect of soil water content, and $F_r(pH)_{DN}^i$ is included to represent the effect of soil pH (this latter was not included in Parton et al., 1996) in the given layer. Importance of pH is highlighted in Wagena et al. (2017).

It is important to note that the equations presented in Wagena et al. (2017) are incorrect. The exact formulae of the equations are much better described in Parton et al. (1996) though their Fig. 5 also contains an error (equation describing the Fr(NO3) has a bracket problem). For clarity, here we provide explicit equations that are error-free according to our best knowledge.

The equation for $F_r(NO_3)$ (Parton et al., 1996):

$$= \left\{ 1 - \left(0.5 + \frac{\text{atan}(\pi \cdot 0.01 \cdot (NO_3^i - 190))}{\pi} \right) \right\} * 25$$

where NO_3 is the nitrate content of the soil expressed in $\mu\text{gN g}^{-1}$ (=ppm).

Effect of soil respiration on the $R_{N_2:N_2O}$ ratio in the given layer:

$$F_r(CO_2)_{DN}^i = 13 + \left(\frac{30.78 \cdot \text{atan}(\pi \cdot 0.07 \cdot (R_{s,tot}^i - 13))}{\pi} \right)$$

where $R_{s,tot}^i$ is total soil respiration (respiration of litter and soil pools) expressed in $\text{kg C ha}^{-1} \text{ day}^{-1}$.

Effect of soil water content status (Parton et al., 1996) in the given layer:

$$F_r(SWC)_{DN}^i = \frac{1.4}{13^{17/pDEN}}$$

$$pDEN = 13^{2.2 \cdot WFPS}$$

$$WFPS^i = \frac{SWC^i}{SWC_{SAT}^i}$$

Effect of soil pH (Wagena et al., 2017) in the given layer:

$$F_r(pH)_{DN}^i = \frac{1}{1470 \cdot e^{-1.1 \cdot pH}}$$

The $R_{N_2:N_2O}$ ratio is used to calculate denitrification related N_2O flux of the given layer from the amount of denitrification (DN) using this formula:

$$F_{N_2O, DN}^i = \frac{DN}{1 + R_{N_2:N_2O} \cdot DNratioN_2O}$$

Denitrification related N_2/N_2O ratio multiplier (DNratioN2O) as a soil input parameter is used to take into account the effect of the soil type (Del Grosso et al., 2000).

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