



## *Supplement of*

# **Simulating measurable ecosystem carbon and nitrogen dynamics with the mechanistically defined MEMS 2.0 model**

**Yao Zhang et al.**

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**Table S1. Summary of the model structure comparison of the new generation process-based soil carbon models.**

Model name	Note	Measurable pools	Simulate N	deep soil C	In vivo/ex vivo pathway	Explicit microbial pool	Rhizosphere and bulk soil	Validated with fractionation data	Reference
BAMS1		Chemical based	N	Y	N	Y	N	N	Riley et al. (2014)
BAMS2	Added nitrogen to BAMS1	Chemical based	Y	Y	N	Y	N	N	Tang et al. (2019)
COMISSI ON		Y	N	Y	Y	Y	N	Y; only one site	Ahrens et al. (2015)
CORPSE		Y	N	Y	N	Y	Y	Y; only two sites	Sulman et al. (2014)
FUN-CORPSE	CORPSE integrated with FUN model	Y	Y	Y	N	Y	Y	N	Sulman et al. (2017)
JSM (Jena Soil Model)	built upon COMISSI ON	Y	Y	Y	Y	Y	N	N	Yu et al. (2020)
MEMS V1		Y	N	N	Y	Y; only litter layer	N	Y	Robertson et al. (2019)
MEMS V2	Full ecosystem model of MEMS V1	Y	Y	Y	Y	Y	Y	Y	This study
MEND		Y	N	N	Y	Y	N	N	Wang et al. (2013)
MEND-CN	Added nitrogen to MEND	Y	Y	N	Y	Y	N	N	Wang et al. (2020)
MIMICS		Y	N	N	N	Y	N	N	Abramoff et al. (2018)
MIMICS		Y	N	N	N	Y	N	N	Wieder et al. (2014)
MIMICS-CN	Added nitrogen to MIMIC	Y	Y	N	N	Y	N	N	Kyker-Snowman et al. (2020)
ORCHIDE E-SOM		N	N	Y	N	N	N	N	Tifafi et al. (2018)
ORCHIMIC		N	Y	N	N	N	N	N	(2018)
SOMic		Y	N	N	Y	Y	N	N	Woolf and Lehmann (2019)
T&C	SOC pools are similar to MEND	Y	Y	N	Y	Y	N	N	Fatichi et al. (2019)

**Table S2. List of major equations in the model. Variable definitions can be found in Tab. S3.**

Equations	Number
<b>Surface litter</b>	
$\frac{dC_{Ssoluble}}{dt} = -C_{Ssoluble} * k_{soluble} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} - C_{Ssoluble} * k_{solubleLeach} * W_{leach} + C_{Shydro} * k_{hydro} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} + C_{Sunhydro} * k_{unhydro} * T_{eff} * W_{eff} * MicCN_{eff} + C_{SmicLitter} * k_{micDeath} * frac_{toSoluble}$	S1
$\frac{dC_{Shydro}}{dt} = -C_{Shydro} * k_{hydro} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} - C_{Shydro} * k_{fragment} * T_{eff} * W_{eff} + C_{SmicLitter} * k_{micDeath} * frac_{toHydro}$	S2
$\frac{dC_{Sunhydro}}{dt} = -C_{Sunhydro} * k_{unhydro} * T_{eff} * W_{eff} * MicCN_{eff} - C_{Sunhydro} * k_{fragment} * T_{eff} * W_{eff} + C_{SmicLitter} * k_{micDeath} * frac_{toUnhydro}$ <p>Note: unlike the soluble and hydrolysable pools, no <math>LCI_{eff}</math> on unhydrolysable pool decay.</p>	S3
$\frac{dC_{SmicLitter}}{dt} = -C_{SmicLitter} * k_{micDeath} + C_{Ssoluble} * k_{soluble} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} * CUE_{Ssoluble}$	S4
$\frac{dC_{SCO2}}{dt} = C_{Ssoluble} * k_{soluble} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} * (1 - CUE_{Ssoluble})$	S5
<b>Rhizosphere litter</b>	
$\frac{dC_{Rsoluble}}{dt} = -C_{Rsoluble} * k_{solubleLeach} * LCI_{eff} + C_{Rhydro} * k_{hydro} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} + C_{Runhydro} * k_{unhydro} * T_{eff} * W_{eff} * MicCN_{eff} + C_{RmicLitter} * k_{micDeath} * frac_{toSoluble}$	S6
$\frac{dC_{Rhydro}}{dt} = -C_{Rhydro} * k_{hydro} * T_{eff} * W_{eff} * LCI_{eff} * MicCN_{eff} - C_{Rhydro} * k_{fragment} * T_{eff} * W_{eff} + C_{RmicLitter} * k_{micDeath} * frac_{toHydro}$	S7
$\frac{dC_{Runhydro}}{dt} = -C_{Runhydro} * k_{unhydro} * T_{eff} * W_{eff} * MicCN_{eff} - C_{Runhydro} * k_{fragment} * T_{eff} * W_{eff} + C_{RmicLitter} * k_{micDeath} * frac_{toUnhydro}$	S8
$\frac{dC_{RDOM}}{dt} = -C_{RDOM} * k_{soluble} * T_{eff} * W_{eff} * MicCN_{eff} - C_{RDOM} * k_{RDOMLeach} * WFPS^3 + C_{Rsoluble} * k_{solubleLeach} * LCI_{eff} + C_{exudate} * k_{exudate}$ <p>Note: the decay rate of surface soluble litter <math>k_{soluble}</math> is also used for RDOM.</p>	S9
$\frac{dC_{RmicLitter}}{dt} = -C_{RmicLitter} * k_{micDeath} + C_{RDOM} * k_{soluble} * T_{eff} * W_{eff} * MicCN_{eff} * CUE_{RDOM}$	S10
$\frac{dC_{RCO2}}{dt} = C_{RDOM} * k_{soluble} * T_{eff} * W_{eff} * MicCN_{eff} * (1 - CUE_{RDOM})$	S11

<p><b>Bulk soil</b></p> $\frac{\partial C_{POM}}{\partial t} = -C_{POM} * k_{POM} * T_{eff} * W_{eff} * MicCN_{eff} + C_{Shydro} * k_{fragment} * T_{eff} * W_{eff} \\ + C_{Sunhydro} * k_{fragment} * T_{eff} * W_{eff} + C_{Rhydro} * k_{fragment} * T_{eff} * W_{eff} \\ + C_{Runhydro} * k_{fragment} * T_{eff} * W_{eff} + C_{micBulk} * k_{micDeath} * frac_{toPOM} \\ + D_{bioturb} \frac{\partial^2(C_{POM})}{\partial Z^2}$ <p>Note: fluxes from surface litter only goes to the POM pool of the first soil layer.</p>	S12
$\frac{\partial C_{DOM}}{\partial t} = -C_{dom} * k_{DOM} * T_{eff} * W_{eff} * MicCN_{eff} - C_{DOM} * k_{adsorpSMAOM} * WFPS^2 \\ * frac_{toSMAOM} - W_{flux} \frac{\partial C_{DOM}}{\partial Z} - k_{adsorpEMAOM} * C_{DOM} * (Sat_{EMAOM} - C_{EMAOM}) \\ + k_{desorpEMAOM} * C_{EMAOM} + C_{micBulk} * k_{micDeath} * (1 - frac_{toPOM}) \\ * (1 - frac_{toSMAOM}) + C_{POM} * k_{POM} * T_{eff} * W_{eff} * MicCN_{eff} + C_{RDOM} \\ * k_{RDOMLeach} * WFPS^3 + D_{diff} \frac{\partial^2(C_{DOM})}{\partial Z^2} + C_{Ssoluble} * k_{solubleLeach} * W_{leach}$ <p>Note: fluxes from surface litter only goes to the DOM pool of the first soil layer.</p>	S13
$\frac{dC_{micBulk}}{dt} = -C_{micBulk} * k_{micDeath} + C_{dom} * k_{dom} * T_{eff} * W_{eff} * MicCN_{eff} * CUE_{DOM} + C_{SMAOM} \\ * k_{SMAOM} * T_{eff} * W_{eff} * MicCN_{eff} * CUE_{SAMOM}$	S14
$\frac{dC_{SMAOM}}{dt} = -C_{SMAOM} * k_{SMAOM} * T_{eff} * W_{eff} * MicCN_{eff} + C_{micBulk} * k_{micDeath} \\ * (1 - frac_{toPOM}) * frac_{toSMAOM} + C_{DOM} * k_{adsorpSMAOM} * WFPS^2 \\ * frac_{toSMAOM}$	S15
$\frac{dC_{BCO2}}{dt} = C_{dom} * k_{DOM} * T_{eff} * W_{eff} * MicCN_{eff} * (1 - CUE_{DOM}) + C_{SMAOM} * k_{SMAOM} * T_{eff} \\ * W_{eff} * MicCN_{eff} * (1 - CUE_{SAMOM})$	S16
$C_{EMAOM} = Sat_{EMAOM} * \frac{lk_{EMAOM} * C_{DOM}}{1 + lk_{EMAOM} * C_{DOM}}$ <p>Note: the Langmuir isotherm was used. It assumes instantaneous equilibrium, resulting in</p> $lk_{EMAOM} = \frac{k_{adsorpEMAOM}}{k_{desorpEMAOM}}$	S17
<p><b>Other</b></p>	
$CUE = micCN_{max} / (CN_{substrate} + CN_{CUE\_km}) \text{ when } CUE \leq CUE_{max}$ $CUE = CUE_{max} \text{ when } CUE > CUE_{max}$	S18
$CN_{substrate} = C_{substrate} / (N_{substrate} + N_{mineral\_avail})$	S19
$frac_{toSMAOM} = (1 - \frac{Sand}{100}) * (1 - \frac{C_{SMAOM}}{Sat_{SMAOM}})$	S20
$lk_{EMAOM} = coeff_{lk} * 10^{-0.186 * pH - 0.216}$	S21
$LCI_{eff} = (LCI_{max} - LCI) / (LCI_{max} - LCI_{min}) \text{ when } LCI \geq LCI_{min}$ $LCI_{eff} = 1 \text{ when } LCI < LCI_{min}$ <p>Note: if <math>LCI_{eff} &lt; LCI_{eff\_min}</math>, then <math>LCI_{eff} = LCI_{eff\_min}</math></p>	S22

$N_{\text{mineral\_demand}} = C_{\text{ssoluble}} * k_{\text{soluble}} * T_{\text{eff}} * W_{\text{eff}} * LCI_{\text{eff}} * MicCN_{\text{eff}} * CUE_{\text{ssoluble}} / micCN_{\text{min}}$ <p>Note: for other pools that used by microbes, similar equations were used.</p>	S23
$Sat_{\text{EMAOM}} = (coeff_{\text{sat1}} * (1 - Sand) + coeff_{\text{sat2}}) * frac_{\text{EMAOMSat}}$	S24
$Sat_{\text{SMAOM}} = (coeff_{\text{sat1}} * (1 - Sand) + coeff_{\text{sat2}}) * (1 - frac_{\text{EMAOMSat}})$	S25
$T_{\text{eff}} = \frac{\frac{\pi}{2} + \text{atan}(coeff_{t1} * (T - coeff_{t2}))}{\pi}$	S26
$W_{\text{eff}} = \frac{1}{1 + coeff_{w1} * e^{(-coeff_{w2} * W_{\text{rel}})}}$	S27
$W_{\text{rel}} = \frac{SWC - SWC_r}{SWC_{FC} - SWC_r} \text{ when } SWC < SWC_{FC}$ $W_{\text{rel}} = 1 \text{ when } SWC \geq SWC_{FC}$	S28

**Table S3. List of variables used in equations in Tab. S2.**

<b>Variable</b>	<b>Definition</b>	<b>Unit</b>
$C_{Ssoluble}$	Carbon in the soluble pool of surface litter	$\text{g C m}^{-2}$
$C_{Shydro}$	Carbon in the hydrolysable pool of surface litter	$\text{g C m}^{-2}$
$C_{Sunhydro}$	Carbon in the unhydrolysable pool of surface litter	$\text{g C m}^{-2}$
$C_{SmicLitter}$	Carbon of the microbial pool in the surface litter	$\text{g C m}^{-2}$
$C_{SCO_2}$	Carbon of the respired $\text{CO}_2$ from the surface litter decomposition	$\text{g C m}^{-2}$
$C_{Rsoluble}$	Carbon in the soluble pool of rhizosphere litter	$\text{g C m}^{-2}$
$C_{Rhydro}$	Carbon in the hydrolysable pool of rhizosphere litter	$\text{g C m}^{-2}$
$C_{Runhydro}$	Carbon in the unhydrolysable pool of rhizosphere litter	$\text{g C m}^{-2}$
$C_{RmicLitter}$	Carbon of the microbial pool in the rhizosphere litter	$\text{g C m}^{-2}$
$C_{RSCO_2}$	Carbon of the respired $\text{CO}_2$ from the rhizosphere litter decomposition	$\text{g C m}^{-2}$
$C_{micBulk}$	Carbon of the microbial pool in the bulk soil	$\text{g C m}^{-2}$
$C_{RDOM}$	Carbon in the rhizosphere DOM pool	$\text{g C m}^{-2}$
$C_{DOM}$	Carbon in the bulk soil DOM pool	$\text{g C m}^{-2}$
$C_{POM}$	Carbon in the bulk soil POM pool	$\text{g C m}^{-2}$
$C_{EMAOM}$	Carbon in the bulk soil exchangeable MAOM pool	$\text{g C m}^{-2}$
$C_{SMAOM}$	Carbon in the bulk soil stable MAOM pool	$\text{g C m}^{-2}$
$C_{exudate}$	Carbon in the root exudate	$\text{g C m}^{-2}$
$C_{BCO_2}$	Carbon of the respired $\text{CO}_2$ from the bulk soil decomposition	$\text{g C m}^{-2}$
$C_{substrate}$	Carbon of the substrate for decomposition	$\text{g C m}^{-2}$
$CN_{substrate}$	C/N ratio of the substrate for decomposition	-
$CN_{CUE\ km}$	Coefficient used to calculate CUE as a function of substrate C/N ratio	-
$CUE$	Carbon use efficiency	-
$CUE_{max}$	Maximum CUE	-
$CUE_{Ssoluble}$	Carbon use efficiency of the surface soluble pool decomposition	-
$CUE_{RDOM}$	Carbon use efficiency of the rhizosphere DOM pool decomposition	-
$CUE_{DOM}$	Carbon use efficiency of the bulk soil DOM pool decomposition	-
$CUE_{SMAOM}$	Carbon use efficiency of the bulk soil stable MAOM pool decomposition	-
$coeff_{sat}$	Two coefficients used for the linear regression that estimates the maximum sorption capacity of soil	-
$coeff_{fk}$	Scaling coefficient used to estimate the binding affinity for the sorption of eMAOM pool	-
$coeff_t$	Two coefficients used to define the temperature effect curve	-
$coeff_w$	Two coefficients used to define the moisture effect curve	-
$D_{bioturb}$	Maximum conductivity used for estimating bioturbation	$\text{cm}^2 \text{ day}^{-1}$
$D_{diff}$	Diffusivity of solute	$\text{cm}^2 \text{ s}^{-1}$
$frac_{toSoluble}$	Fraction of the carbon flow goes to soluble pool	-
$frac_{toHydro}$	Fraction of the carbon flow goes to hydrolysable pool	-
$frac_{toUnhydro}$	Fraction of the carbon flow goes to unhydrolysable pool	-
$frac_{toPOM}$	Fraction of the carbon flow goes to POM	-
$frac_{toSMAOM}$	Fraction of the carbon flow goes to stable MAOM pool	-
$frac_{EMAOMSat}$	Fraction of the maximum sorption capacity of soil that is exchangeable MAOM	-
$k_{soluble}$	Maximum decay rate of soluble litter at optimal temperature and moisture	$\text{day}^{-1}$
$k_{hydro}$	Maximum decay rate of hydrolysable litter at optimal temperature and moisture	$\text{day}^{-1}$
$k_{unhydro}$	Maximum decay rate of unhydrolysable litter at optimal temperature and moisture	$\text{day}^{-1}$
$k_{micDeath}$	Microbial death rate	$\text{day}^{-1}$
$k_{DOM}$	Maximum decay rate of bulk soil DOM at optimal temperature and moisture	$\text{day}^{-1}$
$k_{POM}$	Maximum decay rate of POM at optimal temperature and moisture	$\text{day}^{-1}$
$k_{SMAOM}$	Maximum decay rate of stable MAOM at optimal temperature and moisture	$\text{day}^{-1}$

$k_{exudate}$	Rate of exudate produced by root	$\text{day}^{-1}$
$k_{fragment}$	Maximum fragmentation rate of the litter hydrolysable pool and unhydrolysable pool	$\text{day}^{-1}$
$k_{solubleLeach}$	Maximum rate of soluble litter leached to soil	$\text{day}^{-1}$
$k_{RDOMLeach}$	Maximum rate of rhizosphere DOM leached to bulk soil	$\text{day}^{-1}$
$k_{adsorpSMAOM}$	Maximum rate of DOM adsorption to stable MAOM	$\text{day}^{-1}$
$k_{adsorpEMAOM}$	Rate of DOM adsorption to exchangeable MAOM	$\text{day}^{-1}$
$k_{desorpEMAOM}$	Rate of DOM desorption from exchangeable MAOM	$\text{day}^{-1}$
$LCI$	Lignocellulose index	-
$LCI_{eff}$	Effect of litter LCI on the reaction rate	-
$LCI_{eff\_min}$	Minimum effect on litter decomposition corresponding to $LCI_{min}$	-
$LCI_{max}$	Maximum LCI used in the calculation of LCI effect on litter decomposition	-
$LCI_{min}$	Minimum LCI used in the calculation of LCI effect on litter decomposition	-
$lk_{EMAOM}$	Binding affinity for the sorption of eMAOM pool	$\text{g C day}^{-1}$
$MicCN_{eff}$	Effect of microbial C/N ratio on the reaction rate	-
$micCN_{max}$	Maximum C/N ratio of microbe	-
$micCN_{min}$	Minimum C/N ratio of microbe	-
$N_{substrate}$	Nitrogen of the substrate for decomposition	$\text{g N m}^{-2}$
$N_{mineral\ avail}$	Available mineral N for microbial uptake	$\text{g N m}^{-2}$
$N_{mineral\ demand}$	Microbial demand for mineral N	$\text{g N m}^{-2}$
$pH$	Soil pH	-
$Sand$	Sand content of soil	%
$Sat_{EMAOM}$	Maximum sorption capacity of soil for the exchangeable MAOM	$\text{g C m}^{-2}$
$Sat_{SMAOM}$	Maximum sorption capacity of soil for the stable MAOM	$\text{g C m}^{-2}$
$SWC$	Soil water content	-
$SWC_r$	Residual soil water content	-
$SWC_{FC}$	Soil water content at field capacity	-
$T_{eff}$	Temperature effect	-
$W_{eff}$	Moisture effect	-
$W_{flux}$	Amount of water flows from one soil layer to an adjacent layer	cm
$W_{leach}$	Amount of water flows from litter layer to soil	cm
$W_{rel}$	Relative water content (relative to water holding capacity)	-
$WFPS$	Water filled pore space	-
$z$	Depth from soil surface	cm

**Table S4. List of parameters used in the plant growth submodel.**

Parameter Name	Definition	Unit
perennial_flag	If perennial crop, use 1. For annual crop, use 0.	-
frac_Soluble_Leaf	Fraction of leaf litter allocated to soluble pool	-
frac_Unhydrol_Leaf	Fraction of leaf litter allocated to unhydrolysable pool	-
frac_Soluble_Stem	Fraction of stem litter allocated to soluble pool	-
frac_Unhydrol_Stem	Fraction of stem litter allocated to unhydrolysable pool	-
frac_Soluble_CoarseRoot	Fraction of coarse root litter allocated to soluble pool	-
frac_Unhydrol_CoarseRoot	Fraction of coarse litter allocated to unhydrolysable pool	-
frac_Soluble_FineRoot	Fraction of fine root litter allocated to soluble pool	-
frac_Unhydrol_FineRoot	Fraction of fine root litter allocated to unhydrolysable pool	-
root_water_h1	Matric head above which no water uptake	cm
root_water_h2	Matric head above which water uptake increase from 0 at "root_water_h1" to maximum extraction rate	cm
root_water_h3a	Matric head below which water uptake starts to decrease when potential transpiration rate is very high (0.5 cm/day)	cm
root_water_h3b	Matric head below which water uptake starts to decrease when potential transpiration rate is very low (0.1 cm/day)	cm
root_water_h4	Matric head below which there is no water uptake	cm
bulkDensityLitter	Bulk density of litter	g cm <sup>-3</sup>
litterBio_FullCover	Amount of litter biomass to fully cover the soil.	g m <sup>-2</sup>
wcSaturationLitter	Water content of litter at saturation	-
wcFieldCapacityLitter	Water content of litter at field capacity	-
wcThresLitter	Water content of litter threshold below which evaporation rate cannot meet the potential rate	-
phenoTemperature_Base	Base temperature for phenology	°C
phenoTemperature_Optimum	Optimum temperature for phenology	°C
phenoTemperature_Ceiling	Ceiling temperature for phenology	°C
phenoTemperature_Curvature	Curvature for temperature response for phenology	-
photoPeriodType	Photo period type: 0 for crop type not sensitive to photoperiod, 1 for short-day, 2 for long-day	-
photoPeriod_Critical	Critical photoperiod	hour
photoperiod_Start	Phenology stage when photoperiod sensitive phase start	-
photoperiod_End	Phenology stage when photoperiod sensitive phase end	-
photoPeriodSensitivity	Photo period sensitivity	-
thurnalUnits_Vegetative	Minimum thermal units for vegetative phase	°C
thurnalUnit_Reproductive	Minimum thermal units for reproductive phase	°C
radiationUseEfficiency	Radiation use efficiency (RUE) for total biomass	g biomass MJ PAR <sup>-1</sup>
RUETemperature_Base	Base temperature for RUE	°C
RUETemperature_OptLower	Lower temperature for optimal RUE	°C
RUETemperature_OptUpper	Upper temperature for optimal RUE	°C
RUETemperature_Ceiling	Ceiling temperature for RUE	°C



klight	Light extinction coefficient	-
transp_k_max	Crop coefficient for transpiration at full canopy cover	-
coeff_NitrogenStressRUE	Coefficient for nitrogen stress on RUE	-
specificLeafArea	Specific leaf area	m <sup>2</sup> leaf area g <sup>-1</sup>
rootDepth_max	Maximum rooting depth	cm
rootDepth50	The depth from surface to which 50% of the root mass is distributed.	cm
totalBiomass_init	Initial total biomass at emergence	g m <sup>-2</sup>
frac_ToBlg_init	Fraction of initial biomass that is in root	-
stage_RootFracDecrease	Phenology stage at which allocation fraction of NPP to root reduces	-
stage_RootFracZero	Phenology stage at which allocation fraction of NPP to root is 0	-
frac_BlgToFineRoot_End	Fraction of belowground NPP that is allocated to fine root at the end of root growth state	-
frac_BlgToExudate	Fraction of below ground NPP that is allocated to exudate	-
frac_AbgToLeaf_init	Fraction of aboveground NPP that is allocated to leaf at the beginning of growth	-
Stage_LeafFracDecrease	Phenology stage at which allocation of NPP to leaf is decreasing	-
Stage_LeafFracZero	Phenology stage at which allocation of NPP to leaf is 0	-
GreenLeafWeightRatio_LA_I <sub>max</sub>	Green leaf weight ratio at maximum LAI	-
GreenLeafWeightRatio_PM	Green leaf weight ratio at physiological maturity	-
frac_AbgToStem_DS1	Fraction of aboveground NPP that is allocated to stem at the beginning of reproductive stage	-
Stage_StemFracZero	Phenology stage at which allocation of NPP to stem is 0	-
frac_C_VegOrgan	Carbon content of vegetative organs	g C g biomass <sup>-1</sup>
efficiencyVegOrgan	Growth efficiency for vegetative organs	-
frac_C_Seed	Carbon content of seed	g C g biomass <sup>-1</sup>
efficiencySeed	Growth efficiency for seed	-
LeafNitrogenConc_min	Minimum nitrogen content of leaf	g N g biomass <sup>-1</sup>
StemNitrogenConc_min	Minimum nitrogen content of stem	g N g biomass <sup>-1</sup>
RootNitrogenConc_min	Minimum nitrogen content of coarse and fine root	g N g biomass <sup>-1</sup>
Exudate_NitrogenConc_min	Minimum nitrogen content of exudate	g N g biomass <sup>-1</sup>
SeedNitrogenConc_max	Maximum nitrogen content of seed	g N g biomass <sup>-1</sup>
LeafNitrogenConc_max_DS0	Maximum nitrogen content of leaf at the beginning of growth	g N g biomass <sup>-1</sup>
LeafNitrogenConc_max_DS1	Maximum nitrogen content of leaf at the beginning of reproductive stage	g N g biomass <sup>-1</sup>
StemNitrogenConc_max_fracLeaf	Maximum nitrogen content of stem as a fraction of leaf	g N g biomass <sup>-1</sup>
CoarseRootNitrogenConc_max_fracLeaf	Maximum nitrogen content of coarse root as a fraction of leaf	g N g biomass <sup>-1</sup>
FineRootNitrogenConc_max_fracLeaf	Maximum nitrogen content of fine root as a fraction of leaf	g N g biomass <sup>-1</sup>

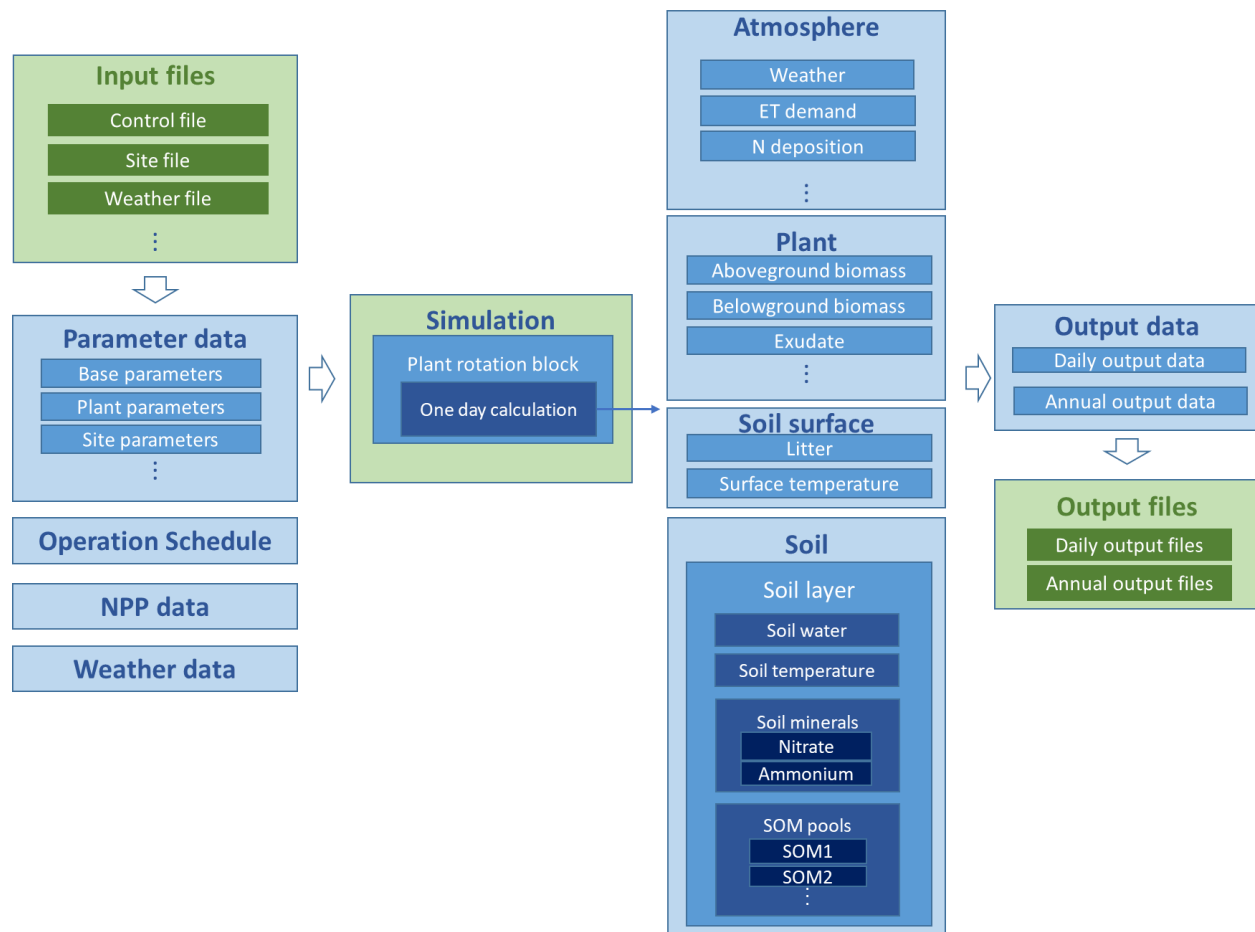
ExudateNitrogenConc_max_fracLeaf	Maximum nitrogen content of exudate as a fraction of leaf	g N g biomass <sup>-1</sup>
Stage_CoarseRootDeath_start	Phenology stage at which coarse root start to die	-
frac_CoarseRootDeath	Death rate of coarse root	day <sup>-1</sup>
frac_FineRootDeath	Death rate of fine root	day <sup>-1</sup>
Stage_StemDeath_start	Phenology stage at which stem start to die	-
frac_StemDeath	Death rate of stem	day <sup>-1</sup>
Stage_tanslocToSeed_start	Phenology stage at which translocation of nitrogen to seed starts	-
Coeff_transloc	Coefficient for nitrogen translocation to seed	day <sup>-1</sup>
frac_stem_senescence	Rate of stem becomes senescence at the end of growing season for perennials	day <sup>-1</sup>
frac_root_senescence	Rate of root becomes senescence at the end of growing season for perennials	day <sup>-1</sup>
frac_stem_storage	Maximum fraction of stem is storage of carbohydrate that can be used for regrowth from defoliation and initial growth at the beginning of a growing season	day <sup>-1</sup>
ratio_ShootRoot_crit	The critical shoot root ratio below which more photosynthate is allocated aboveground	-
frac_StandingDeadFall	Rate of standing dead biomass falls to become litter	day <sup>-1</sup>

**Table S5. Sources of the input data for model simulations of the NEON sites.**

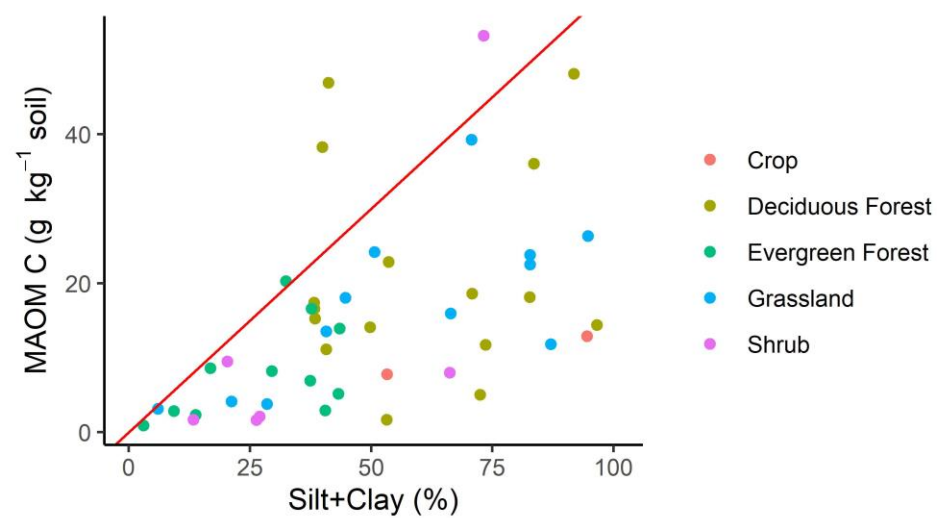
<b>Input data</b>	<b>Source</b>	<b>Reference</b>
Weather	High Plains Regional Climate Center database; SCAN database	<a href="https://hprcc.unl.edu/">https://hprcc.unl.edu/</a> (accessed on 02/13/2020); Schaefer et al. (2007)
Historical fire frequency	Historical fire frequency map	Guyette et al. (2012)
Recent fire frequency and time	NEON database	NEON (2020e)
Total atmospheric N deposition	Total atmospheric N deposition map	Hember (2018)
Biological N fixation	Regression on actual ET	Cleveland et al. (1999)
Actual ET for calculation of Biological N fixation	MODIS Land Subset Products	<a href="https://modis.ornl.gov/">https://modis.ornl.gov/</a> (accessed on 05/12/2020); ORNL DAAC (2018); Running et al. (2017)
NPP	MODIS Land Subset Products	<a href="https://modis.ornl.gov/">https://modis.ornl.gov/</a> (accessed on 05/12/2020); ORNL DAAC (2018); Running et al. (2015)
Water potentials for root water uptake	Field measurements	(2001)
C and N removed from fire	Field measurements	Ojima (1990)
Aboveground and belowground C allocation	Aboveground and belowground NPP maps	Bradford et al. (2005)
Soil physical property	NEON database	NEON (2020)
Soil chemical property	NEON database	NEON (2020b)
Plant aboveground physical and chemical properties	NEON database	NEON (2020c)
Root chemical properties	NEON database	NEON (2020d)

**Table S6. Soil properties for the Soil Climate Analysis Network (SCAN) sites used for soil water and temperature validation.**

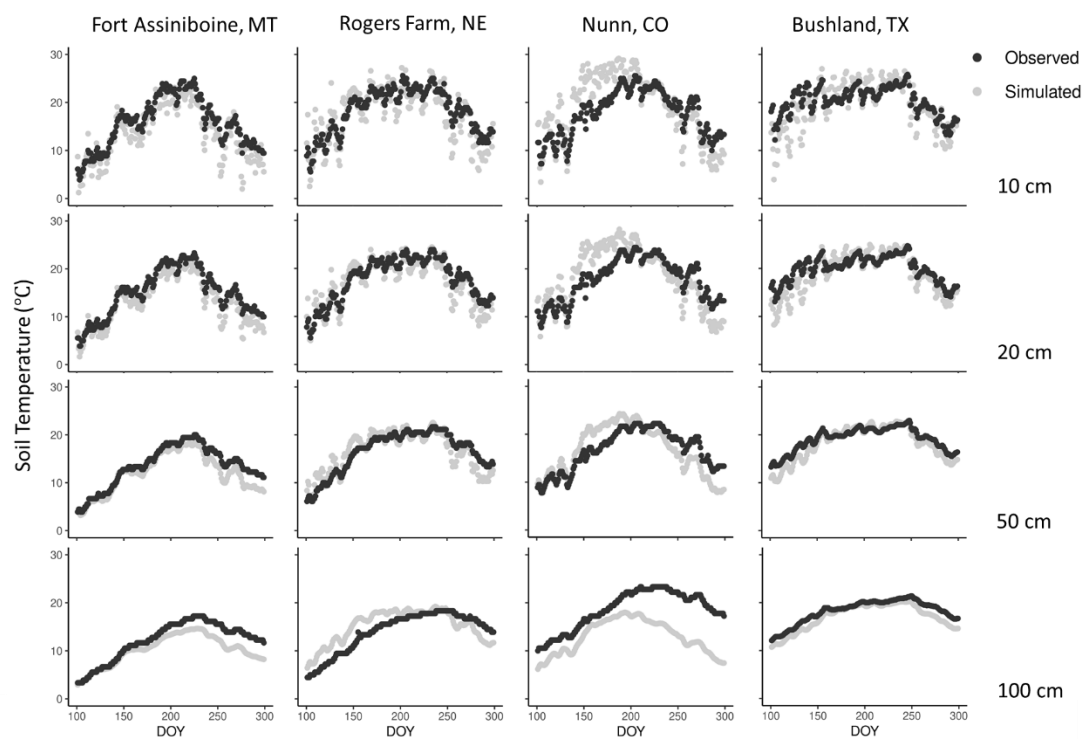
	<b>Bushland, TX</b>	<b>Fort Assiniboine, MT</b>	<b>Nunn, CO</b>	<b>Rogers Farm, NE</b>
<b>0 – 20 cm</b>				
Sand (%)	21.2	33.4	70.6	6.5
Clay (%)	27.0	22.6	17.6	36.0
Bulk Density (g cm <sup>-3</sup> )	1.3	1.3	1.5	1.4
Organic C (%)	2.5	1.3	0.9	2.3
<b>20 – 50 cm</b>				
Sand (%)	15.5	27.8	73.3	4.3
Clay (%)	45.3	29.9	17.1	41.9
Bulk Density (g cm <sup>-3</sup> )	1.4	1.3	1.6	1.3
Organic C (%)	0.8	0.9	0.4	1.1
<b>50 – 100 cm</b>				
Sand (%)	14.8	36.0	73.4	4.2
Clay (%)	39.8	23.7	16.2	36.8
Bulk Density (g cm <sup>-3</sup> )	1.5	1.6	1.5	1.4
Organic C (%)	0.4	0.4	0.1	0.4



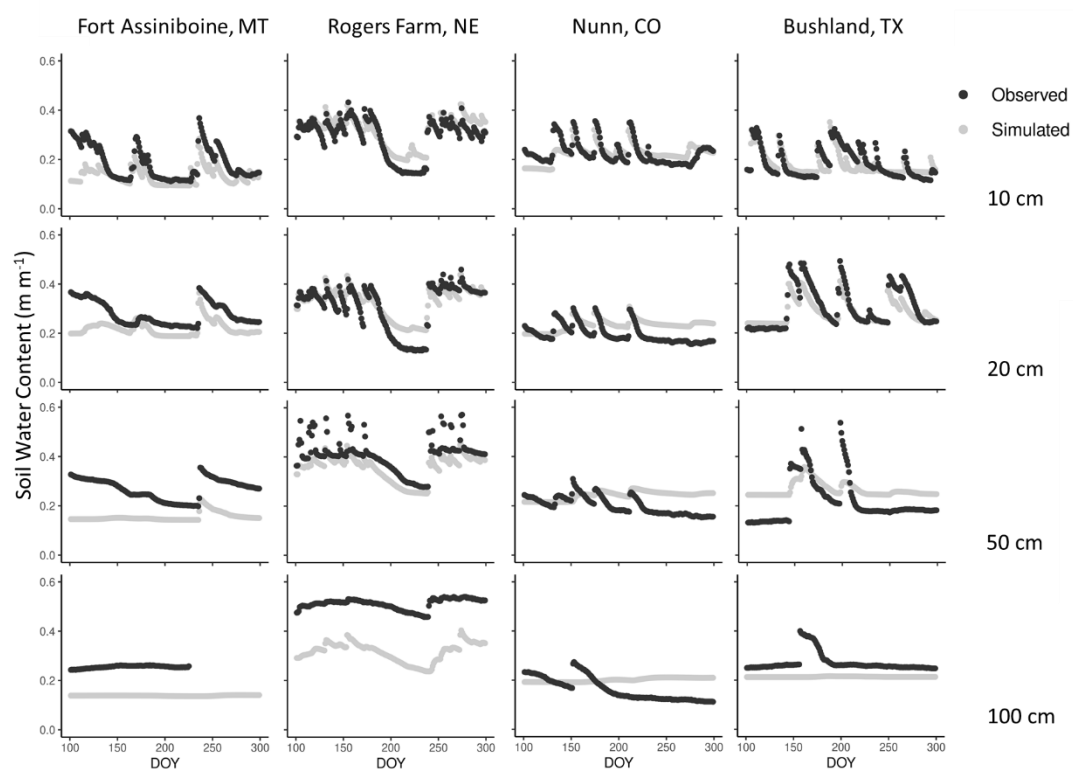
**Figure S1.** The structure of the model in Java. Each box represents one or a set of objects in Java.



**Figure S2.** The fitted saturation curve using measured mineral-associated (MAOM) carbon from this study and soil texture data from the NEON database.

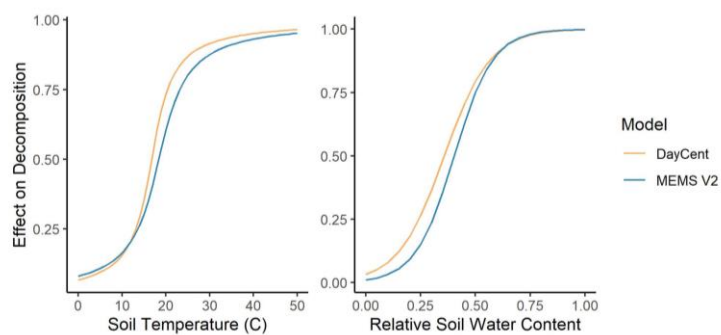


**Figure S3.** An example of simulated soil temperature in comparison with measurements of four Soil Climate Analysis Network (SCAN) sites. Daily average data in 2014 were presented. The statistics can be found in Table 4.



**Figure S4.** An example of simulated soil water content in comparison with measurements of four Soil Climate Analysis Network (SCAN) sites. Daily average data in 2014 were presented. The statistics can be found in Table 4.





**Figure S5.** The calibrated curves for temperature and moisture effect on decomposition used in the MEMS 2.0 model. The curves are compared with those in the DayCent model.

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# Simulating measurable ecosystem carbon and nitrogen dynamics with the mechanistically defined MEMS 2.0 model

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