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Diffusion limitations and Michaelis–Menten kinetics as drivers of combined temperature and moisture effects on carbon fluxes of mineral soils

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Model M2-dif steady state equations

The equilibrium solutions to the C pools of model M2-dif are given by:

$$C_P = K_D r_{ed} z(-2gI_{ml}f_{ge}f_{ug}r_{md} + 2gI_m f_{ug}r_{md} - 2gI_{sl}f_{ge}r_{mr}f_{ug} - 2gI_{sl}f_{ge}f_{ug}r_{md} + 2gI_{sl}r_{mr} + 2gI_{sl}r_{md} - I_{ml}f_{ge}f_{ug}r_{ed}r_{md} + I_{ml}f_{ug}r_{ed}r_{md} - I_{sl}f_{ge}r_{mr}f_{ug}r_{ed} - I_{sl}f_{ge}f_{ug}r_{ed}r_{md} + I_{sl}r_{mr}r_{ed} + I_{sl}r_{ed}r_{md})/(gI_{ml}V_D f_{ge}r_{mr}f_{ug} + gI_{ml}V_D f_{ge}f_{ug}r_{md} + 2gI_{ml}f_{ge}f_{ug}r_{ed}r_{md} - 2gI_{ml}f_{ug}r_{ed}r_{md} + gI_{sl}V_D f_{ge}r_{mr}f_{ug} + gI_{sl}V_D f_{ge}f_{ug}r_{md} + 2gI_{sl}f_{ge}r_{mr}f_{ug}r_{ed} + 2gI_{sl}f_{ge}f_{ug}r_{ed}r_{md} - 2gI_{sl}r_{mr}r_{ed} - 2gI_{sl}r_{ed}r_{md} + I_{ml}f_{ge}f_{ug}r_{ed}^2 r_{md} - I_{ml}f_{ug}r_{ed}^2 r_{md} + I_{sl}f_{ge}r_{mr}f_{ug}r_{ed}^2 + I_{sl}f_{ge}f_{ug}r_{ed}^2 r_{md} - I_{sl}r_{mr}r_{ed}^2 - I_{sl}r_{ed}^2 r_{md}) \qquad (S1)$$

$$C_D = -z(r_{mr} + r_{md})/(gV_U f_{ug}(f_{ge} - 1)) \qquad (S2)$$

$$C_M = f_{ug}(I_{ml}f_{ge} - I_{ml} + I_{sl}f_{ge} - I_{sl})/(f_{ge}r_{mr}f_{ug} - r_{mr} + f_{ug}r_{md} - r_{md}) \qquad (S3)$$

$$C_{ED} = -gf_{ge}f_{ug}(I_{ml}r_{mr} + I_{ml}r_{md} + I_{sl}r_{mr} + I_{sl}r_{md})/(r_{ed}(2gf_{ge}r_{mr}f_{ug} - 2gr_{mr} + 2gf_{ug}r_{md} - 2gr_{md} + f_{ge}r_{mr}f_{ug}r_{ed} - r_{mr}r_{ed} + f_{ug}r_{ed}r_{md} - r_{ed}r_{md})) \qquad (S4)$$

$$C_{EM} = -f_{ge}f_{ug}(gI_{ml}r_{mr} + gI_{ml}r_{md} + gI_{sl}r_{mr} + gI_{sl}r_{md} + I_{ml}r_{mr}r_{ed} + I_{ml}r_{ed}r_{md} + I_{sl}r_{mr}r_{ed} + I_{sl}r_{ed}r_{md})/(r_{ed}(2gf_{ge}r_{mr}f_{ug} - 2gr_{mr} + 2gf_{ug}r_{md} - 2gr_{md} + f_{ge}r_{mr}f_{ug}r_{ed} - r_{mr}r_{ed} + f_{ug}r_{ed}r_{md} - r_{ed}r_{md})) \qquad (S5)$$

In these equations, I_{ml} and I_{sl} are metabolic and structural litter input, which represent litter additions to the C_D and C_P pools, respectively.

Supplementary figures

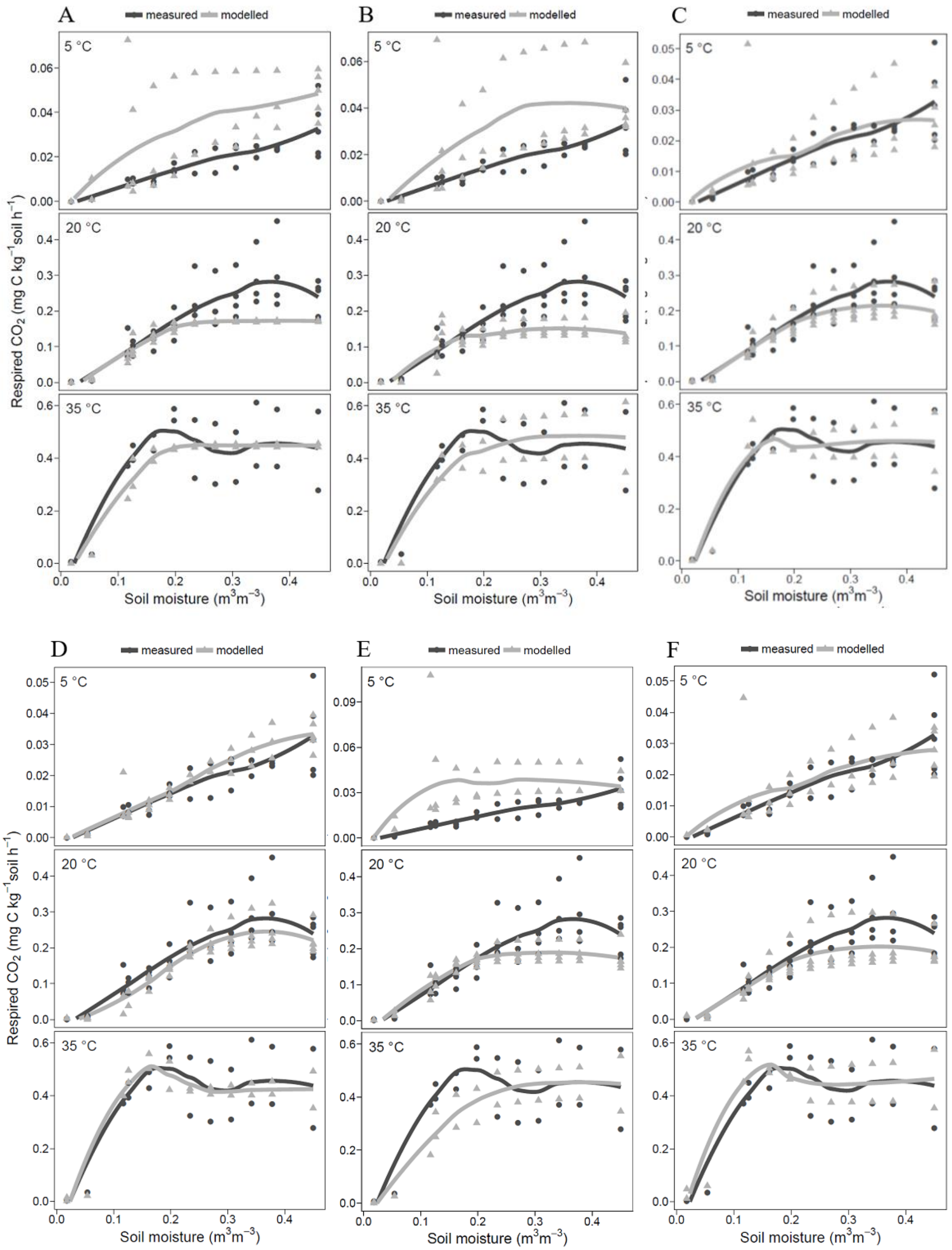

Figure S1: The relationship between respiration rates and soil moisture content shown for observations and diffusion based models with different reaction kinetics. Each plot compares the measurements with a different model. A: 11-dif, B: 22-dif, C: M1-dif, D: M2-dif, E: MM-dif, and F: Mr2-dif. The average relationship is depicted with smooth loess fits.

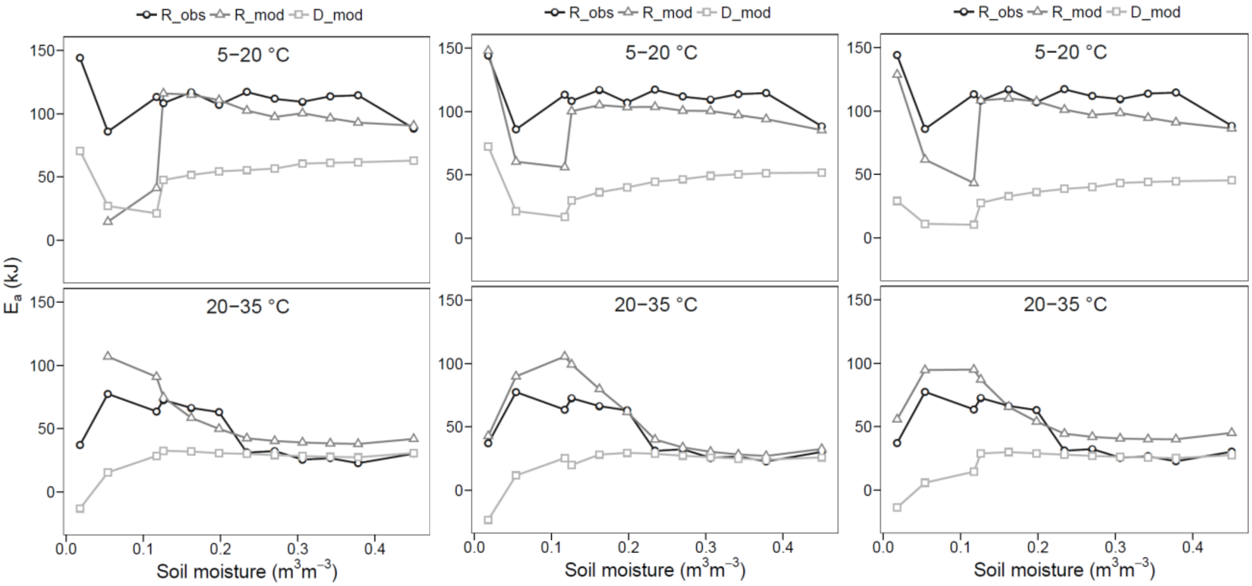

Figure S2: The relationship between apparent temperature sensitivities and soil moisture content shown for observations and M1-dif (left), M2-dif (middle) and M$_r$2-dif (right).

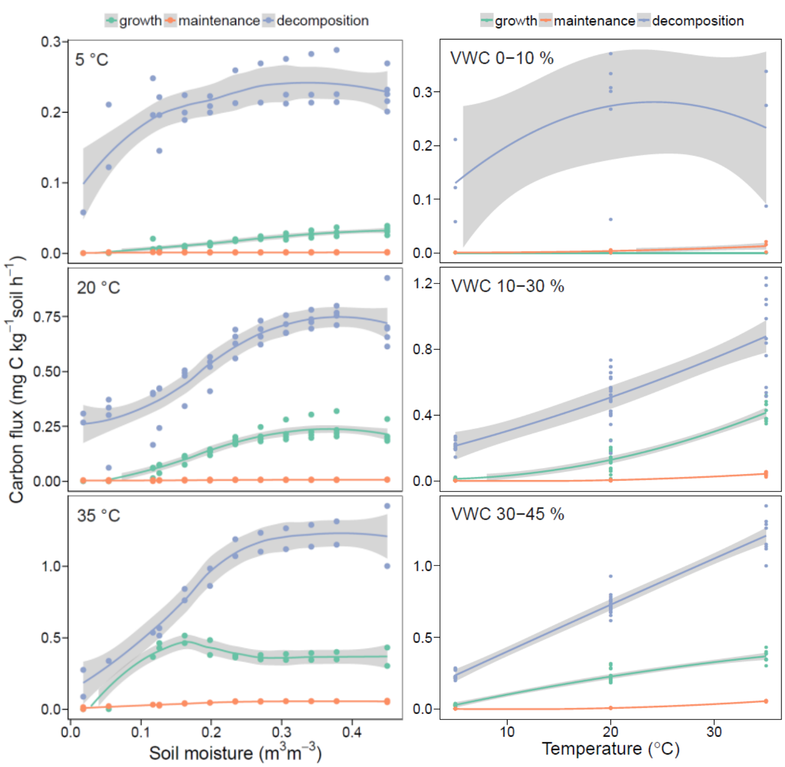

Figure S3: Modelled growth respiration, maintenance respiration and decomposition against soil moisture (left plot) and soil temperature (right plot) using model M2-dif.

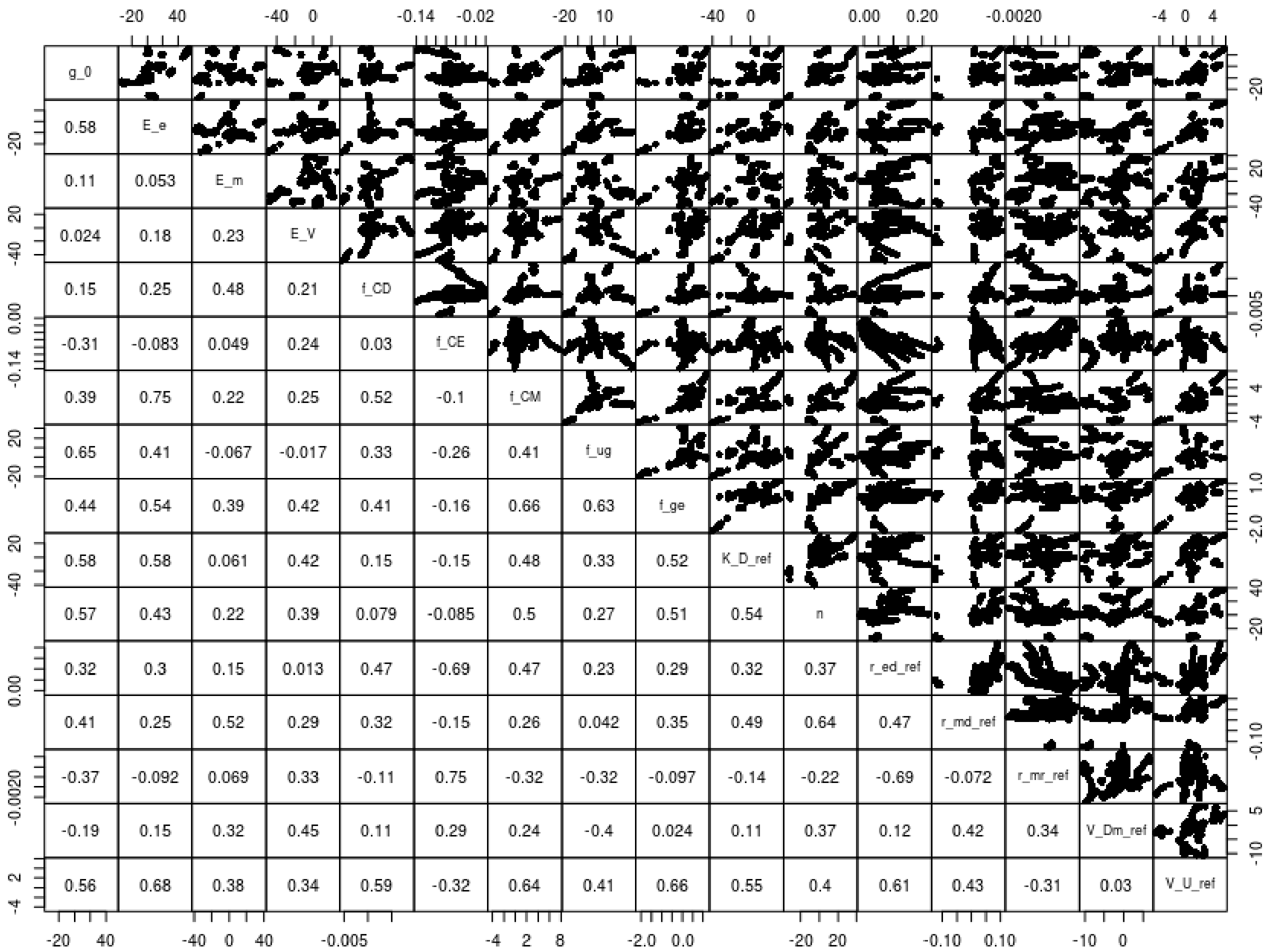

Figure S4: Correlations between sensitivity functions of model parameters (from R function sensFun, package FME). Parameters resulting in 0 sensitivity (*n*, θ_{th}) are excluded.

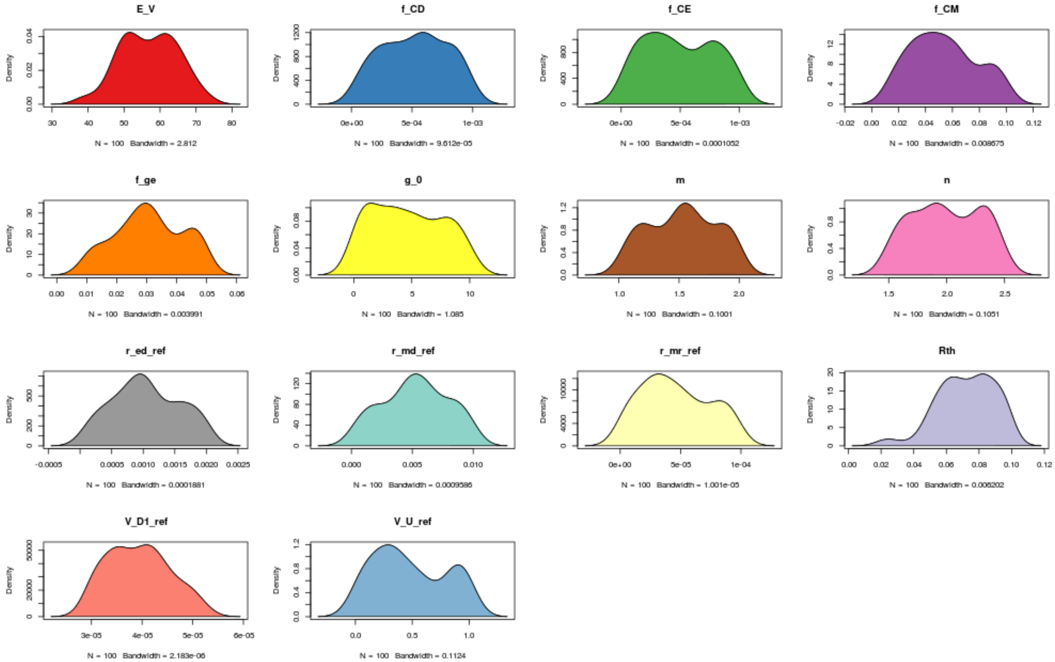

Figure S5: Kernel density estimations for model 11-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

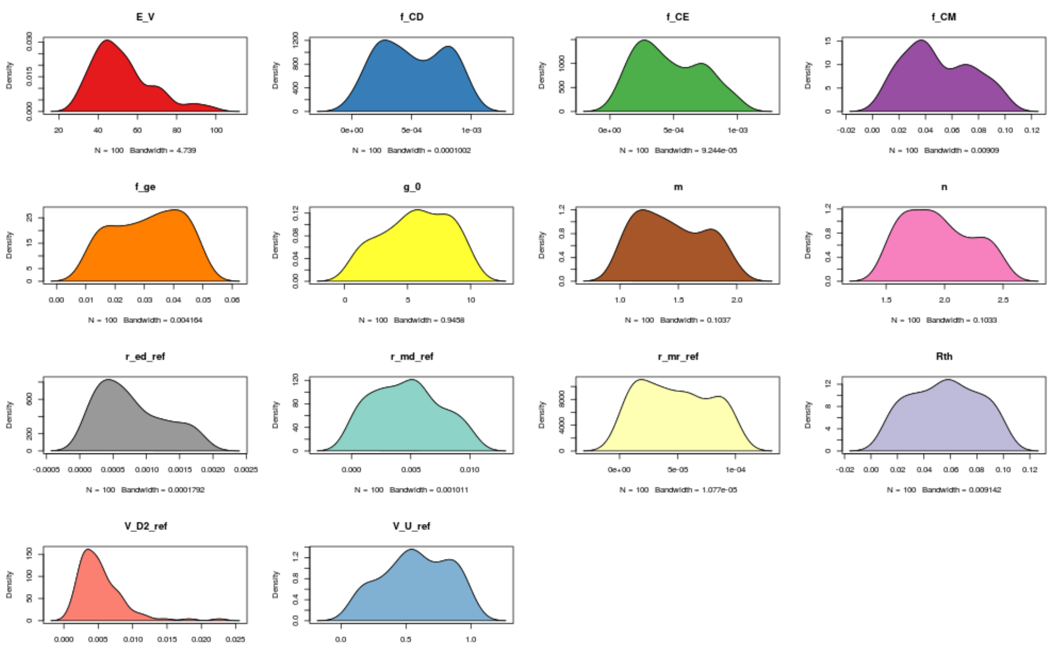

Figure S6: Kernel density estimations for model 22-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

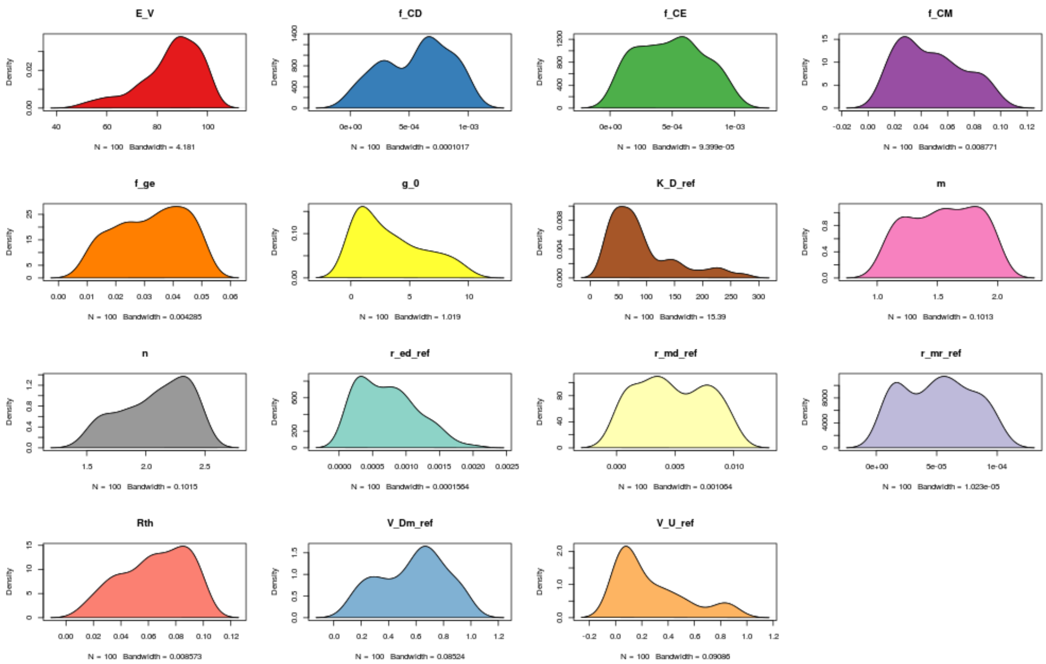

Figure S7: Kernel density estimations for model M1-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

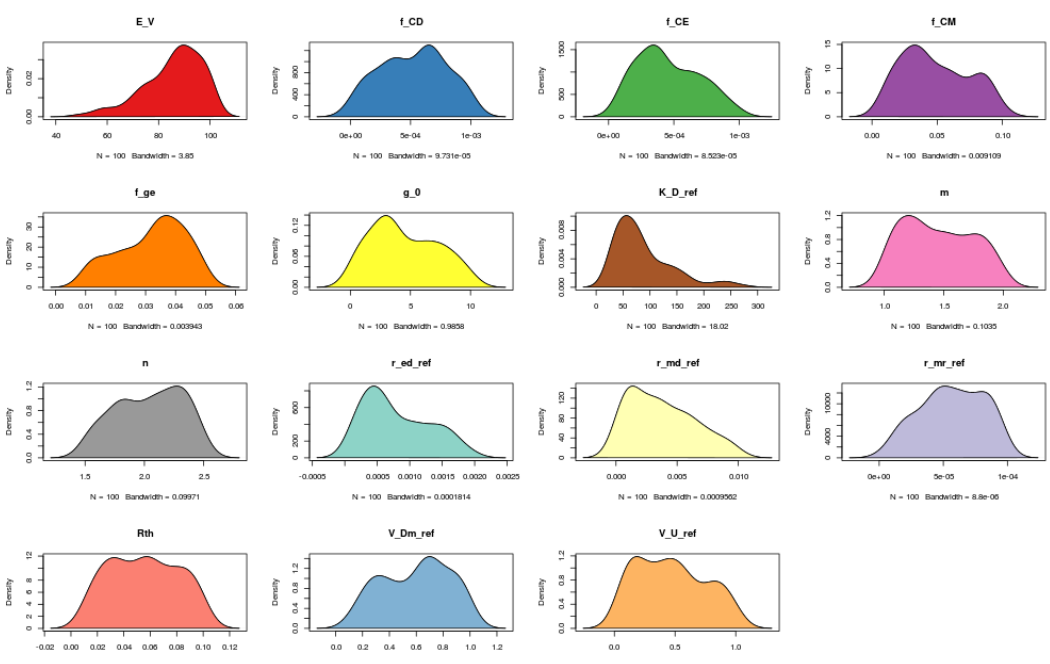

Figure S8: Kernel density estimations for model M2-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

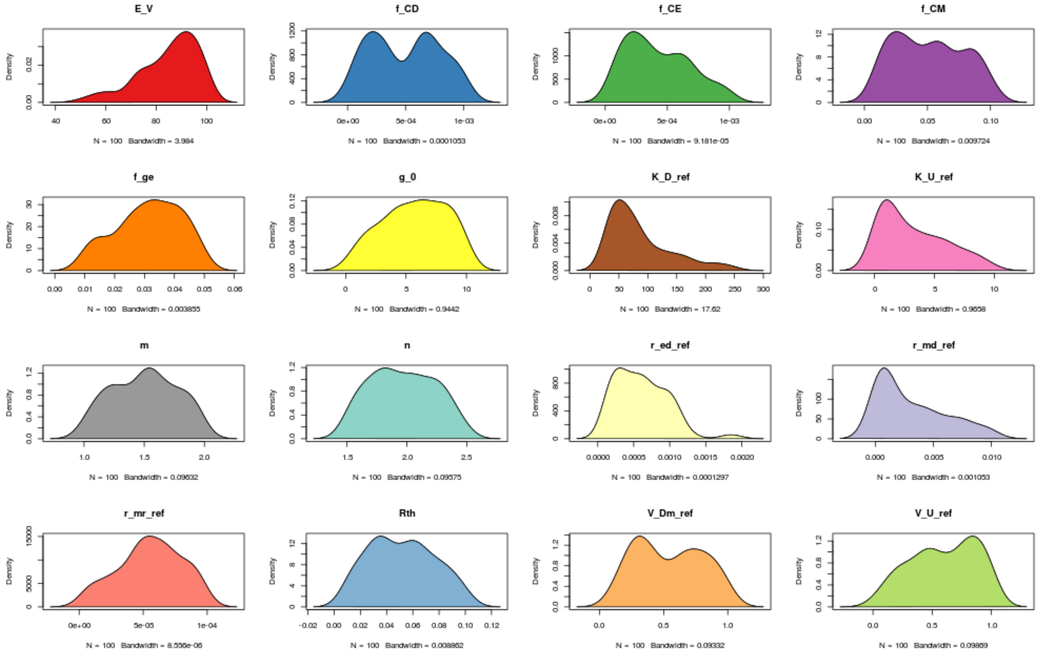

Figure S9: Kernel density estimations for model MM-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

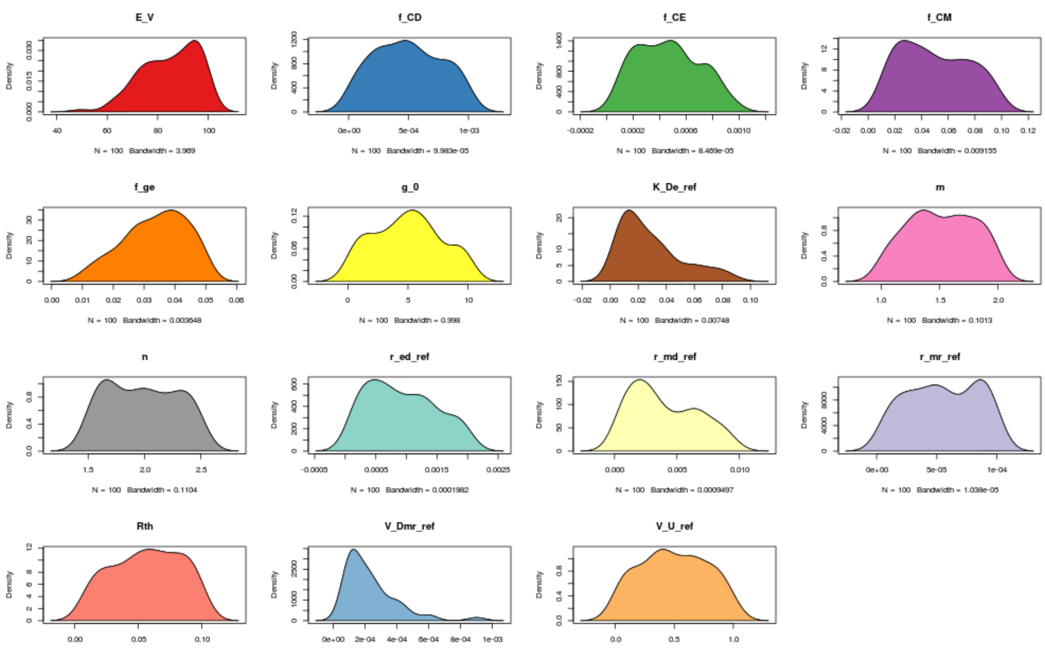

Figure S10: Kernel density estimations for model M_r2-dif. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

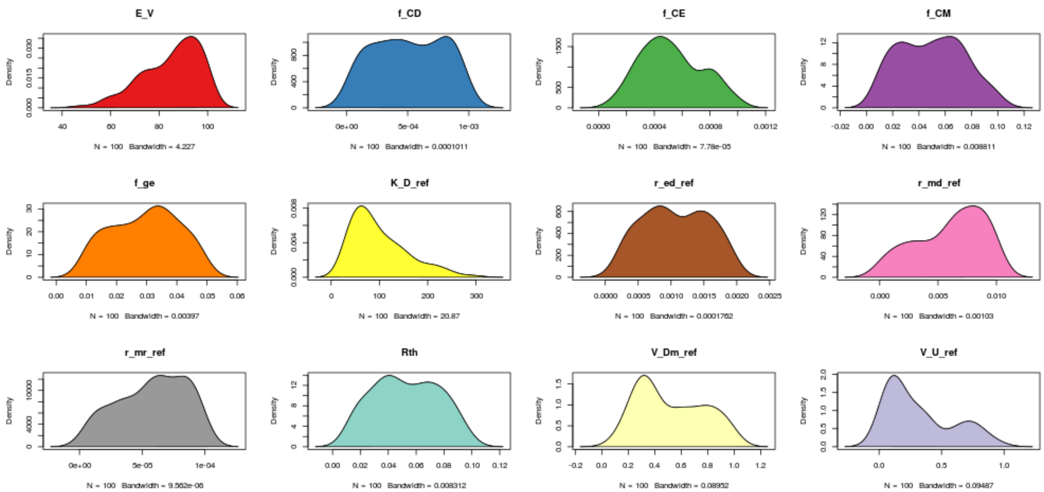

Figure S11: Kernel density estimations for model M2-psi. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

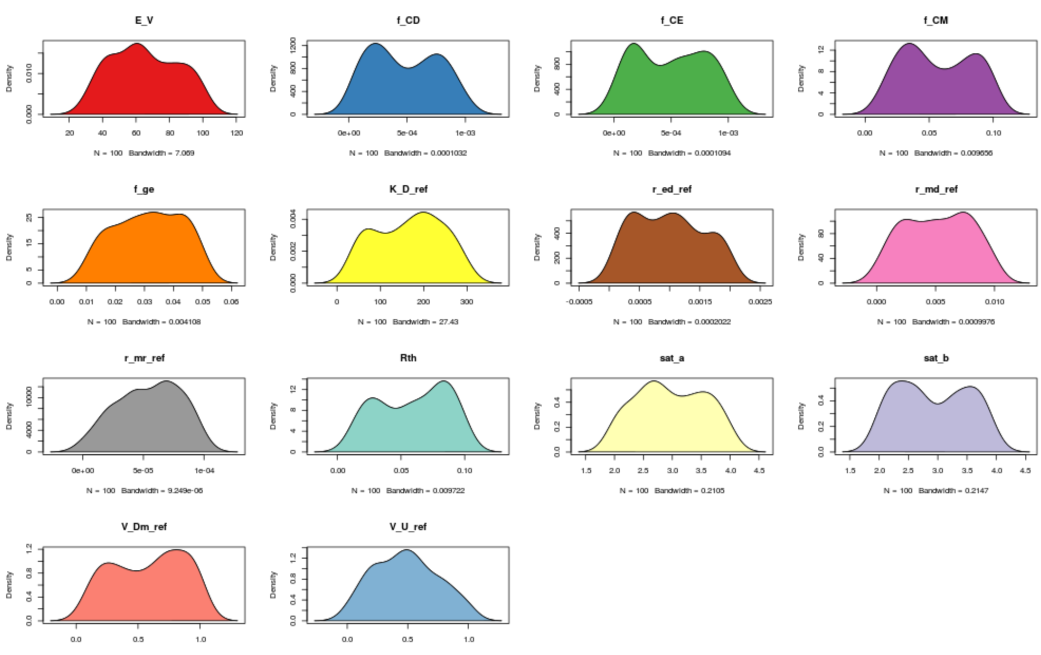

Figure S12: Kernel density estimations for model M2-sat. Estimations are made with the 100 parameter sets resulting in the lowest model cost from 30000 (Latin Hypercube).

Supplementary tables

Table S1: Calibrated model parameters with lower and upper bounds.

Symbol	Description	Units	Lower	Upper	References
E_V	Activation energy for VD_ref, VU_ref, rmr_ref, KD	kJ	30	100	(Price and Sowers, 2004; Tang and Riley, 2014; Wang et al., 2013)
f_D	Initial CD fraction of SOC	kg kg^{-1}	1.00E-05	0.001	-
f_E	Initial CEM, CED fraction of SOC	kg kg^{-1}	1.00E-05	0.001	-
f_M	Initial CM fraction of SOC	kg kg^{-1}	0.01	0.1	-
f_{ge}	Fraction of growth going to CEM	kg kg^{-1}	0.01	0.05	(Schimel and Weintraub, 2003)
g_0	Conductance for diffusion	h-1	0.1	10	(Hu and Wang, 2003; Jones et al., 2005; Manzoni et al., 2016; Vetter et al., 1998)
K_{D_ref}	Michaelis-Menten constant of decomposition Eq. (8)	kg C m^{-3}	30	300	-
K_{De_ref}	Michaelis-Menten constant of decomposition Eq. (9)	kg C m^{-3}	0.001	0.1	-
K_{U_ref}	Michaelis-Menten constant of uptake Eq. (8)	kg C m^{-3}	0.01	10	-
m	Exponent in Eq. (11)	-	1	2	(Hamamoto et al., 2010)
n	Exponent in Eq. (11)	-	1.5	2.5	(Hamamoto et al., 2010)
r_{ed_ref}	Reference rate of CEM, CED decay	h-1	0.0001	0.002	(Li et al., 2014)
r_{md_ref}	Reference rate of CM decay	h-1	0.0001	0.01	(Li et al., 2014)
r_{mr_ref}	Reference rate of maintenance respiration	h-1	1.00E-06	0.0001	(Price and Sowers, 2004)
θ_{th}	Moisture threshold for diffusion	m^3 m^{-3}	0.01	0.1	(Manzoni and Katul, 2014)
a	Moisture function coefficient Eq. (21)	-	2	4	(Moyano et al., 2013)
b	Moisture function coefficient Eq. (21)	-	2	4	(Moyano et al., 2013)
V_{D1_ref}	Reference rate of decomposition Eq. (6)	h-1	1.00E-05	0.001	(Li et al., 2014)
V_{D2_ref}	Reference rate of decomposition Eq. (7)	h-1	0.001	0.1	(Li et al., 2014)
V_{Dm_ref}	Reference rate of decomposition Eq. (8)	h-1	0.1	1	(Li et al., 2014)
V_{Dmr_ref}	Reference rate of decomposition Eq. (9)	h-1	1.00E-05	0.001	(Li et al., 2014)
V_{U_ref}	Reference rate of carbon uptake	h-1	0.01	1	(Li et al., 2014)

Table S2: Fixed model parameters.

Symbol	Description	References	Value	Units
E_e	Activation energy for r_{ed_ref}	(Grisi et al., 1998; Salazar-Villegas et al., 2016)	10	kJ
E_m	Activation energy for r_{md_ref}	(Grisi et al., 1998; Salazar-Villegas et al., 2016)	10	kJ
f_{ug}	Fraction of uptake to growth (i.e. CUE)	(Hagerty et al., 2014)	0.7	kg kg^{-1}
pd	Particle density	-	2700	kg m^{-3}
Ψ_{opt}	Optimal water potential Eq. (22)	-	33	kPa
Ψ_{th}	Threshold water potential Eq. (22)	-	15000	kPa
R	R gas constant	-	0.0083	-
T_{ref}	Reference temperature Eq. (20)	-	290	°K
sand	Soil sand fraction	-	0.28	kg kg^{-1}
silt	Soil silt fraction	-	0.57	kg kg^{-1}
clay	Soil clay fraction	-	0.15	kg kg^{-1}
ps	Soil pore space	-	0.45	m^3 m^{-3}
toc	Soil total organic carbon	-	0.012	kg
z	Soil depth	-	1	m
Ψ_{sat}	Saturation water potential	-	0.46	kPa

Table S3: Calibrated model parameters showing optimal values found for each model version. A missing value means the parameter was not part of the model.

Par	11-dif	22-dif	M1-dif	M2-dif	MM-dif	M2-psi	M2-sat	Mr2-dif
E_V	49	39	99	94	98	68	94	94
f_D	0.00014	2.50E-05	4.00E-05	9.10E-05	5.10E-05	0.00096	0.00018	0.001
f_E	9.20E-05	0.00021	0.00071	0.00068	0.00041	0.00057	0.00066	0.00042
f_M	0.092	0.012	0.085	0.08	0.012	0.015	0.065	0.042
f_{ge}	0.048	0.018	0.041	0.034	0.018	0.031	0.031	0.033
g_0	1.1	9	5.6	0.98	8.3	-	-	0.61
K_{D_ref}	-	-	53	62	31	100	180	-
K_{De_ref}	-	-	-	-	-	-	-	0.063
K_{U_ref}	-	-	-	-	1.1	-	-	-
m	1.9	1.1	1.3	1.1	1.7	-	-	1
n	2.4	2.3	2.3	2.3	2.5	-	-	2.2
r_{ed_ref}	0.0018	0.00056	0.00038	0.00056	0.00017	0.0016	0.00064	0.00025
r_{md_ref}	0.0087	0.0096	0.0036	0.00099	0.0016	0.0093	0.008	0.00059
r_{mr_ref}	5.50E-06	9.70E-05	8.90E-05	1.50E-05	9.80E-05	9.00E-05	8.80E-05	4.80E-05
θ_{th}	0.029	0.055	0.049	0.063	0.011	-	-	0.06
a	-	-	-	-	-	-	3.1	-
b	-	-	-	-	-	-	2.1	-
V_{D1_ref}	4.80E-05	-	-	-	-	-	-	-
V_{D2_ref}	-	0.0082	-	-	-	-	-	-
V_{Dm_ref}	-	-	0.23	0.37	0.22	0.65	0.57	-
V_{Dmr_ref}	-	-	-	-	-	-	-	0.00028
V_{U_ref}	0.082	0.75	0.018	0.11	0.19	0.11	0.15	0.18

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