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An improved process-oriented hydro-biogeochemical model for simulating dynamic fluxes of methane and nitrous oxide in alpine ecosystems with seasonally frozen soils

Wei Zhang et al.

Correspondence to: Xunhua Zheng (xunhua.zheng@post.iap.ac.cn)

Supplementary materials

Table S1 The equations of soil thermal module in CNMM-DNDC

Equation	Description	Remark
$C\frac{\partial T}{\partial t}=\frac{\partial}{\partial Z}(k\frac{\partial T}{\partial Z})$	Heat conduction	Solved by implicit method of Crank-Nicholson
$C_l = C_{l,\ OM}\theta_{l,\ OM} + C_{l,\ Min}\theta_{l,\ Min} + C_{l,\ Water}\theta_{l,\ Water} + C_{l,\ Air}\theta_{l,\ Air}$	Heat capacity	
$k_l = a_l + (b_l - a_l) \times \text{Depth}_l$	Thermal conductivity	
a_l	Constant for thermal conductivity	
	$\text{Depth}_l < 0.2$ m	0.34 (dimensionless)
	0.2 m $\leq \text{Depth}_l < 1.0$ m	1.5 (dimensionless)
	$\text{Depth}_l \geq 1.0$	1.69 (dimensionless)
b_l	Constant for thermal conductivity	
	$\text{Depth}_l < 0.2$ m	0.58 (dimensionless)
	0.2 m $\leq \text{Depth}_l < 1.0$ m	2.05 (dimensionless)
	$\text{Depth}_l \geq 1.0$	3.63 (dimensionless)

$C_{l,\ OM}$, $C_{l,Min}$, $C_{l,\ Water}$, and $C_{l,\ Air}$ are the heat capacity of organic matter, minerals, water and air. $\theta_{l,\ OM}$, $\theta_{l,\ Min}$, $\theta_{l,\ Water}$, $\theta_{l,\ Ice}$, $\theta_{l,\ Air}$ is the relative volumetric fraction of each constituent in the soil. Depth is the depth of soil layer.

Table S2 Information about the observed data for model validation.

Item	Period	Ecosystem	Instruments	Data provider
Soil temperature	2013.11−2014.11 2014.06−2015.10 2014.04−2015.04	Wetland Meadow Forest	Temperature loggers (StowAway TidbiT v2, Onset Computer Co., USA	H Zhang Z Yao, H Zhang Z Yao
Soil moisture	2013.11−2014.11 2014.06−2015.10 2014.04−2015.04	Wetland Meadow Forest	Digital thermometer (JM624, Tianjin JM Instrument Co. Ltd., China)	H Zhang Z Yao, H Zhang Z Yao
Methan flux	2013.11−2014.11 2013.11−2014.11 2014.04−2015.04	Wetland Meadow Forest	Static opaque chambers for air sampling and a gas chromatography for air sample analysis	H Zhang Z Yao, H Zhang Z Yao
Nitrous oxide flux	2013.11−2014.11 2013.11−2014.11 2014.04−2015.04	Wetland Meadow Forest		H Zhang Z Yao, H Zhang Z Yao

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Table S3 Input settings of the CNMM-DNDC for the three alpine ecosystems in the Rierlangshan catchment based on measurement and investigation.

Input	Depth (cm)	Alpine wetland	Alpine meadow	Alpine forest
Soil property				
Bulk density ($g\ cm^{-3}$)	0−10	0.3	0.9	0.9
	10-20	0.5	0.9	0.9
	20−40	0.8	1.0	0.9
	40−100	1.1	1.2	1.2
Organic carbon ($g\ kg^{-1}$)	0−10	307.7	63.5	153.0
	10-20	283.4	50.0	113.0
	20−40	254.3	37.0	73.0
	40−100	299.9	19.0	23.0
Total nitrogen ($g\ kg^{-1}$)	0−10	18.2	4.8	9.4
	10-20	13.2	3.8	7.5
	20−40	12.0	3.0	4.8
	40−100	15.2	1.5	2.0
Clay content (<0.002 mm) (0–1)	0−10	0.03	0.23	0.07
	10-20	0.04	0.26	0.08
	20−40	0.04	0.24	0.11
	40−100	0.04	0.24	0.12
Silt content (0.002–0.05 mm) (0–1)	0−10	0.64	0.64	0.78
	10-20	0.64	0.64	0.72
	20−40	0.67	0.67	0.72
	40−100	0.66	0.66	0.75
pH	0−10	6.8	6.7	7.2
	10-20	6.8	6.4	7.2
	20−40	6.8	6.6	7.2
	40−100	6.8	6.8	7.2
Vegetation type		Wetland (*Kobresia humilis*)	Meadow (*Deschampsia littoralis*)	Forest (Coniferous tree)
Mangement of Graze		2013/11/29−2013/12/20 2014/06/04−2014/07/07 2014/10/12−2014/11/06	2013/11/29−2013/12/20 2014/06/04−2014/07/07 2014/10/12−2014/11/11	
Graze intensity (sheep unit $ha^{-1}\ yr^{-1}$)		1.48	1.48	

Table S4 The pedo-transfer functions used in this study.

$$K_s = 2.2\times10^{-7}\, e^x \quad (1)$$

$$x = 7.755 + 0.0352\mathrm{si} - 0.967\mathrm{bd}^2 - 0.000484\mathrm{cl}^2 - 0.000322\mathrm{si}^2 + 0.001/\mathrm{si} - 0.0748/\mathrm{som} - 0.643\ln(\mathrm{si}) - 0.01398\,\mathrm{bd}\cdot\mathrm{cl} - 0.1673\mathrm{bd}\cdot\mathrm{som}$$

$$\mathrm{FC} = 0.85\times(1-\mathrm{bd}/2.65) - 0.06\mathrm{bd}^2$$

$$\mathrm{WP} = (150/a)^{1.0/b} \quad (2)$$

$$a = e^{-4.396 - 7.15\times10^{-2}\,\mathrm{cl} - 4.88\times10^{-4}\,\mathrm{sa}^2 - 4.285\times10^{-5}\,\mathrm{sa}^2\,\mathrm{cl}} \quad (3)$$

$$b = -3.14 - 2.22\times10^{-3}\,\mathrm{cl}^2 - 3.484\times10^{-5}\,\mathrm{sa}^2\cdot\mathrm{cl} \quad (4)$$

In Eqs. 1–6, x, a and b are the intermediate variables involved in the calculation of *K*s or WP. *K*s is in the unit of m s^{-1}, WP are expressed in volumetric content (%), bd denotes bulk density in g cm^{-3}, som is soil organic matter content in %, and cl, si, and sa denote clay (< 0.002 mm), silt (0.002–0.05 mm), and sand (0.05–2 mm) fractions in %, respectively.

Table S5 Equations for the statistical criteria for model valiation.

$$\text{IA} = 1 - \frac{\sum_{k=1}^{n} (s_k - o_k)^2}{\sum_{k=1}^{n} (|s_k - \bar{o}| + |o_k - \bar{o}|)^2} \quad \text{(S1)}$$

$$\text{NSE} = 1 - \frac{\sum_{k=1}^{n} (o_k - s_k)^2}{\sum_{k=1}^{n} (o_k - \bar{o})^2} \quad \text{(S2)}$$

$$R^2 = 1 - \frac{\sum_{k=1}^{n} (o_k - \hat{o}_k)^2}{\sum_{k=1}^{n} (o_k - \bar{o})^2} \quad \text{(S3)}$$

$$s = \text{slope} \times o \text{ (ZIR equation)} \quad \text{(S4)}$$

In Eqs. S1−4, IA, NSE and R^2 are abbreviations of the index of agreement, Nash–Sutcliffe index, and the determination coefficient of the zero-intercept univariate linear regression of the observations against the simulations, k and n (k = 1, 2..., n) denote the kth pair and the total pair number of the values, respectively; s and o denote the simulation and observation, respectively; $\bar{o}$ represents the mean of the observations (o); $\hat{o}$ is the prediction using the regression; and slope is the slope of the zero-intercept univariate linear regression (ZIR) of the observations against the simulations. These equations are given by referring to Nash and Sutcliffe (1970), Willmott and Matsuurra (2005), Moriasi et al. (2007), Jiang (2010), Congreves et al. (2016) and Dubache et al. (2019).

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Table S6 Equations and parameters used in the module of denitrification for the CNMM-DNDC

Equations of denitrification

Equations	Description	
$GR_{ONx} = GR_{ONx}(\max) \times \frac{[DOC]}{K_C + [DOC]} \times \frac{[ON_X]}{K_N + [ON_X]}$	Growth rate of each denitrifiers	Eq. 1
$GR = F_T \times (GR_{NO3} \times PH1 + GR_{NO2} \times PH2 + GR_{NO} \times PH3 + GR_{N_2O} \times PH3$	Growth rate of all denitrifiers	Eq. 2
$PH1 = 0.4 \times (pH - 2.5)$	Effects of soil pH for NO_3^-	Eq. 3
$PH2 = 0.4 \times (pH - 3.0)$	Effects of soil pH for NO_2^-	Eq. 4
$PH3 = 0.4 \times (pH - 3.5)$	Effects of soil pH for NO and N_2O	Eq. 5
$(\frac{dBIO_d}{dt})_{growth} = GR \times BIO_d$	Growth of denitrifiers	Eq. 6
$(\frac{dBIO_d}{dt})_{death} = M_C \times Y_C \times BIO_d$	Death of denitrifiers	Eq. 7
$\frac{dC}{dt} = (\frac{GR}{Y_C} + M_C) \times BIO_d$	Consumption of organic carbon	Eq. 8
$\frac{dON_X}{dt} = (\frac{GR_{ONx}}{Y_{ONx}} + M_{ONx} \times \frac{[ON_X]}{N}) \times BIO_d$	Consumption of nitrogen substrates	Eq. 9
$(\frac{dN}{dt})_{assi} = (\frac{dBIO_d}{dt})_{growth} / CN$	Assimilation of nitrogen	Eq. 10
$F_T = a \times 2^{\frac{T_{soil} - 22.5}{10.0}}$	Effects of soil temperature	Eq. 11

Parameters of the equations

Symbol	Description	value	Unit
K_c	Semi-saturation constant of dissolved organic carbon	0.017	kg C m^{-3}
K_N	Semi-saturation constant of NO_3^-, NO_2^-, NO and N_2O	0.083	kg N m^{-3}
$GR_{NO3(max)}$	Maximum growth rate constant of NO_3^- denitrifiers	0.67	h^{-1}
$GR_{NO2(max)}$	Maximum growth rate constant of NO_2^- denitrifiers	0.67	h^{-1}
$GR_{NO(max)}$	Maximum growth rate constant of NO denitrifiers	0.34	h^{-1}
$GR_{N2O(max)}$	Maximum growth rate constant of N_2O denitrifiers	0.34	h^{-1}
CN	Carbon to nitrogen ratio of denitrifiers	3.45	dimensionless
M_c	Maintenance coefficient of dissolved organic carbon	0.0076	kg C kg^{-1} h^{-1}
$M_{(NO3)}$	Maintenance coefficient of NO_3^-	0.09	kg N kg^{-1} C h^{-1}
$M_{(NO2)}$	Maintenance coefficient of NO_2^-	0.035	kg N kg^{-1} C h^{-1}
$M_{(NO)}$	Maintenance coefficient of NO	0.079	kg N kg^{-1} C h^{-1}
$M_{(N2O)}$	Maintenance coefficient of N_2O	0.079	kg N kg^{-1} C h^{-1}
Y_c	Maximum increase rate of DOC	0.503	kg C kg^{-1} C
$Y_{(NO3)}$	Maximum increase rate of NO_3^-	0.401	kg C kg^{-1} N
$Y_{(NO2)}$	Maximum increase rate of NO_2^-	0.428	kg C kg^{-1} N
$Y_{(NO)}$	Maximum increase rate of NO	0.151	kg C kg^{-1} N
$Y_{(N2O)}$	Maximum increase rate of N_2O	0.151	kg C kg^{-1} N

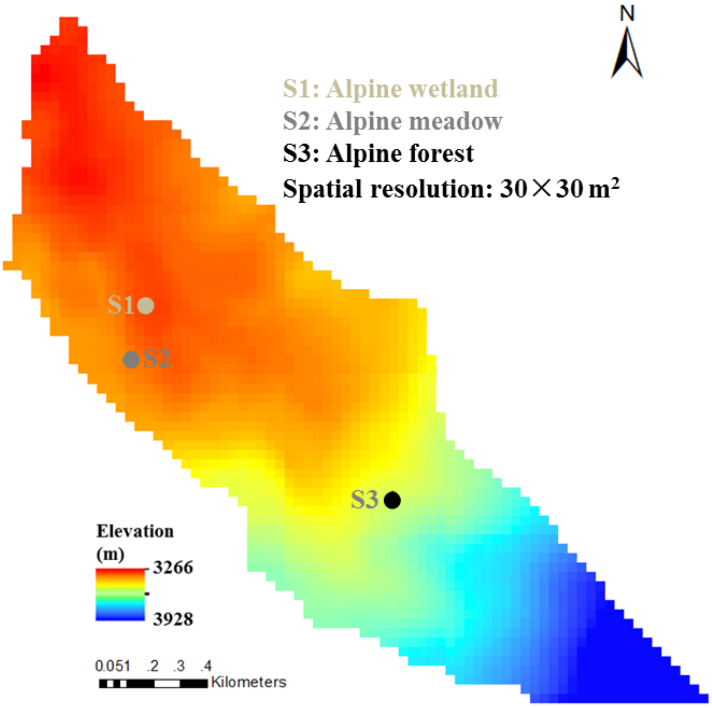

Figure: S1 The digital elevation model (DEM) of the Rierlangshan catchment (data from Geospatial Data Cloud; http://www.gscloud.cn/) with the sites of field observations.

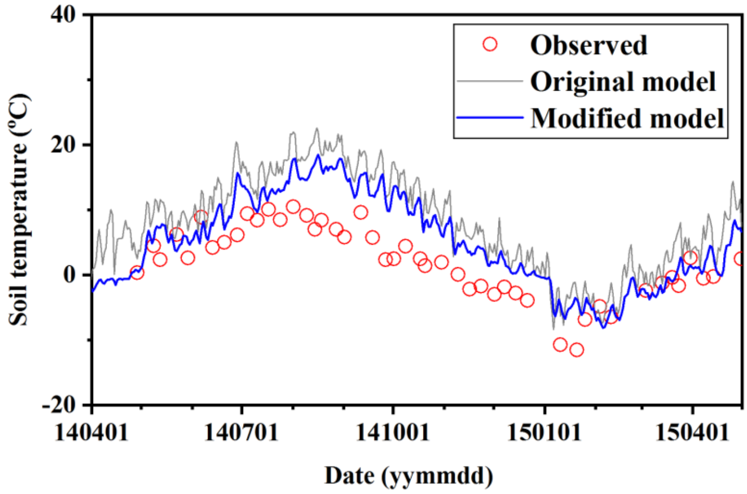

Figure: S2 Observed and simulated daily topsoil (5 cm) temperature from alpine forest by both the original and modified models.

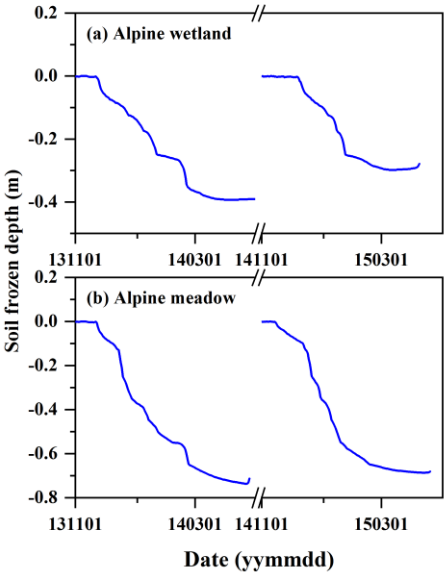

Figure: S3 The simulated dynamics of soil frozen depth dynamics from alpine wetland and alpine meadow.

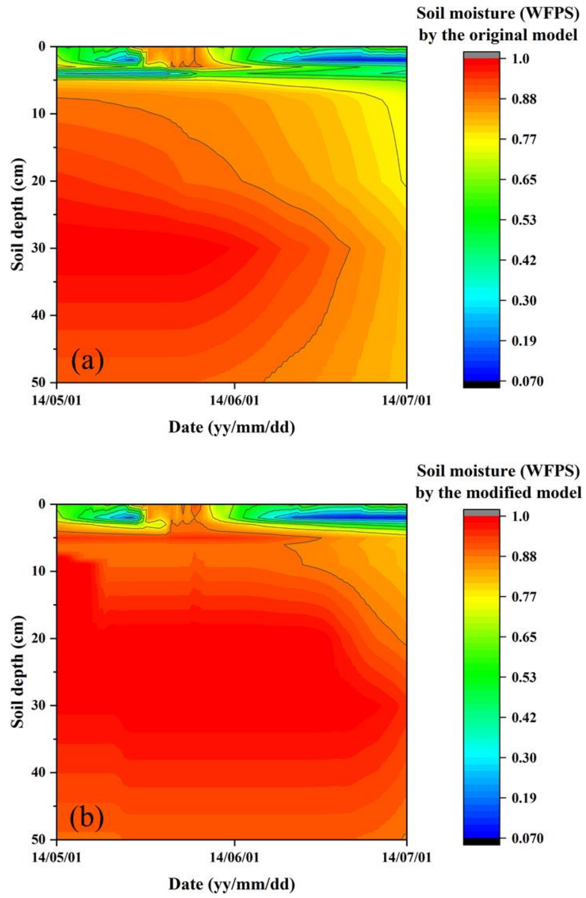

Figure: S4 The simulated soil profile moisture by the original and modified models for the alpine wetland.