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

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16 Abstract. The hydro-biogeochemical model Catchment Nutrient Management Model - DeNitrification-DeComposition 17 (CNMM-DNDC) was established to simultaneously quantify ecosystem productivity and losses of nitrogen and carbon at the 18 site or catchment scale. As a process-oriented model, this model is expected to be universally applied to different climate 19 zones, soils, land uses and field management practices. This study is one of many efforts to fulfil such an expectation, which 20 was performed to improve the CNMM-DNDC by incorporating a physical-based soil thermal module to simulate the soil 21 thermal regime in the presence of freeze-thaw cycles. The modified model was validated with simultaneous field 22 observations in three typical alpine ecosystems (wetlands, meadows and forests) within a catchment located in the seasonally 23 frozen region of the eastern Tibetan Plateau, including soil profile temperature, topsoil moisture and fluxes of methane  $(CH_4)$ 24 and nitrous oxide (N<sub>2</sub>O). The validation showed that the modified CNMM-DNDC was able to simulate the observed 25 seasonal dynamics and magnitudes of above variables in the three typical alpine ecosystems, with index of agreement values 26 of 0.91-1.00, 0.49-0.83, 0.57-0.88 and 0.26-0.47, respectively. Consistent with the emissions determined from the field 27 observations, the simulated aggregate emissions of  $CH_4$  and  $N_2O$  were highest for the wetland among three alpine 28 ecosystems, which were dominated by the  $CH_4$  emissions. This study indicates the possibility for utilizing the process-29 oriented model CNMM-DNDC to predict hydro-biogeochemical processes, as well as related gas emissions, in seasonally 30 frozen regions. As the original CNMM-DNDC was previously validated in some unfrozen regions, the modified CNMM-31 DNDC could be potentially applied to estimate the emissions of  $CH_4$  and  $N_2O$  from various ecosystems under different 32 climate zones at the site or catchment scale.

## 33 1 Introduction

34 During the last 50 years, the extraordinary changes in the nitrogen and carbon cycles have occurred globally, which are 35 essential components of ecosystems (e.g., Galloway et al., 2008; Canfield et al., 2010). Climate changes due to warming and 36 human anthropogenic activities derived from food production have significantly altered the cycling of nitrogen and carbon 37 and led to increased reactive nitrogen availability and carbon losses, which result in a series of environmental problems at 38 the catchment, regional and even global scales (e.g., Galloway et al., 2004; Galloway et al., 2008; Ju et al., 2009). Excessive 39 reactive nitrogen in soils can be lost in the forms of nitrogen gases, such as nitrous oxide (N<sub>2</sub>O), nitric oxide (NO) and 40 ammonia (NH<sub>3</sub>), and nitrogen pollution, such as nitrate (NO<sub>3</sub><sup>-</sup>) and ammonium (NH<sub>4</sub><sup>+</sup>), in water through leaching or surface 41 runoff (e.g., Seitzinger, 2008; Collins et al., 2016). In the face of increased air temperatures and intensive land use changes, 42 especially in cold regions, the soil organic carbon stored since the Last Glacial Maximum has been lost to the atmosphere via 43 methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>) (e.g., Piao *et al.*, 2009; Fenner and Freeman, 2011; Schuur *et al.*, 2015). These 44 nitrogen and carbon losses contribute to potential global warming (CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O), air pollution (NO and NH<sub>3</sub>) and surface/groundwater pollution ( $NO_3^-$  and  $NH_4^+$ ). Therefore, sustainable ecosystems urgently need to be established that not 45 46 only focus on net primary productivity but also are friendly to the environment with the minimal hazards, including 47 greenhouse gases, air pollution and water pollutants (e.g., Cui et al., 2018; Zhang et al., 2019).

48 The cycling of nitrogen and carbon is closely related to soil water processes (e.g., Breuer et al., 2010; Vereecken et al., 49 2016; Zhang et al., 2018b). Thus, interactions among soil waters and the cycling of nitrogen and carbon govern biological 50 productivity and environmental outcomes (e.g., Zhu *et al.*, 2018). The interactions consist of the redox potential for different 51 transformation processes influenced by the spatiotemporal variation in soil water content and the lateral transport of water 52 and dissolved nitrogen or carbon controlled by surface and subsurface flow (e.g., McClain et al., 2003; Castellano et al., 53 2013; Bechmann, 2014). For example, the variation in soil water content can create hot spots or moments of nitrogen and carbon losses by influencing plant nitrogen uptake, redox potential, and the transport of dissolved nitrogen and carbon (e.g., 54 55 Zhu et al., 2012; Keiluweit et al., 2017). Therefore, a complete understanding of biogeochemical processes will inevitably 56 involve interactions among soil water and the cycling of nitrogen and carbon (e.g., Breuer et al., 2010; Vereecken et al., 57 2016; Zhu et al., 2018).

58 Biogeochemical models, such as DNDC, LandscapeDNDC, WNMM, MOMOS, CENTURY and DayCent, are 59 effective tools for simulating the cycling of nitrogen and carbon and quantifying the effects of climate change and 60 anthropogenic activities on ecosystems (e.g., Foereid et al., 2007; Haas et al., 2012; Li, 2007; Li et al., 2007; Pansu et al., 61 2010; Cheng et al., 2014; Pansu et al., 2014). In recent years, some new conceptual approaches are applied in the 62 biogeochemical models, such as centering on the functional role of the soil microbial biomass (Pansu et al., 2010; Pansu et 63 al., 2014) and detailing the lateral transport of water and nutrients (Haas et al., 2012; Zhang et al., 2018b). Generally, 64 comprehensive hydrological processes, especially for the lateral transport of water and nutrients, are simplified or ignored in 65 most models due to specific questions that must be addressed (e.g., Li, 2007; Li et al., 2007; Chen et al., 2008; Deng et al., 66 2014). For the land surface or hydrological models at large scales, they are designed with explicit mechanisms of hydrology 67 and generally focus on vertical and lateral nutrient transport, such as nitrate loads into rivers (e.g., Liu *et al.*, 2019). However, 68 the simulations of nitrogen and carbon processes are usually based on empirical functions even without predicting gas loss. 69 Due to the various purposes of different models, coupling soil hydrological models with biogeochemical models can be an 70 effective strategy for integrating soil water and cycling of nitrogen and carbon to improve model performance. Thus, the 71 coupled model with improved performance can be applied to simultaneously predict productivity and potential negative 72 environmental effects (e.g., Chen *et al.*, 2008; Zhu *et al.*, 2018).

73 In recent years, efforts have been implemented to couple models, such as SWAT-N, LandscapeDNDC-CMF, APSIM, 74 SWAT-DayCent, and CNMM-DNDC (e.g., Pohlert et al., 2007; Haas et al., 2012; Holzworth et al., 2014; Wu et al., 2016; 75 Zhang et al., 2016; Zhang et al., 2018b). The models derived from SWAT were all based on semi-distributed hydrological 76 models using hydrologic response units and did not perform better in estimating non-point source pollution (e.g., Pohlert et 77 al., 2007; Bosch et al., 2011; Wu et al., 2016). A coupler was used to couple two models for LandscapeDNDC-CMF, which 78 realized the simulation of horizontal movement of water and nutrients (e.g., Haas et al., 2012; Klatt et al., 2017; Schroeck et 79 al., 2019). Compared with other models, the Catchment Nutrient Management Model - DeNitrification-DeComposition 80 (CNMM-DNDC), which was established by incorporating the core biogeochemical processes of DNDC into the hydrological framework of the CNMM, was validated at a catchment with complex landscapes in the subtropical region and 81 82 showed good performance for simultaneously simulating various variables, including ecosystem productivity, hydrological 83 nitrogen losses and nitrate discharge in streams, and emissions of gaseous carbon and nitrogenous gases (Zhang et al., 84 2018b). Therefore, the CNMM-DNDC has the capacity to simulate the various variables closely related to both productivity 85 and environmental hazards.

86 However, as a process-oriented hydro-biogeochemical model designed to be applicable to different climate zones, soils, 87 land uses and field management practices, CNMM-DNDC testing is still lacking due to limited observations for model 88 validation. In this study, the model was applied to a catchment in a seasonally frozen region located on the eastern Tibetan 89 Plateau with the land use types of alpine wetlands, meadows and forests to test its ability to simulate hydro-biogeochemical 90 processes. However, scientific descriptions of soil thermal dynamics due to freeze-thaw cycles are still lacking for the CNMM-DNDC. This gap may hinder model application in seasonally frozen regions, which account for 56% of the exposed 91 92 land surface of the Northern Hemisphere (Jiang et al., 2020). In addition, the soil freeze-thaw cycles that occur in these mid-93 high latitude regions exert important influences on soil thermal dynamics, as well as on related hydrological processes, thus 94 increasing the availability of substrates and stimulating the processes of  $CH_4$  and  $N_2O$  production and emissions in soils (e.g., 95 Song et al., 2019). Therefore, we hypothesize that adding the missing scientific processes of soil thermal dynamics into the internal model program codes can improve the performance of the CNMM-DNDC in simulating the soil thermal dynamics, 96 97 hydrological processes and  $CH_4$  and N<sub>2</sub>O fluxes in seasonally frozen regions. Filling this gap is especially necessary to 98 broaden model applicability.

99 To test the above hypothesis, the catchment simulation in the Rierlangshan was conducted using a unique experimental 100 dataset, which was obtained by Zhang et al. (2018a, 2019) and Yao et al. (2019) for the catchment that involved three typical 101 alpine ecosystems, wetlands, meadows and forests, on the eastern Tibetan Plateau. The aims of this study were to (i) attempt to address the gap in the CNMM-DNDC by improving the scientific processes of soil thermal dynamics for seasonally 102 103 frozen regions and (ii) compare the performances of the original and modified models in simulating the soil profile 104 temperature, topsoil moisture and  $CH_4$  and  $N_2O$  fluxes in three typical alpine ecosystems in the Rierlangshan catchment with 105 field observations. Therefore, the validated model with modifications provides a mechanism for not only interpreting 106 observations but also predicting the  $CH_4$  and  $N_2O$  fluxes in alpine ecosystems.

## 107 2 Materials and methods

#### 108 2.1 Model description

# 109 2.1.1 Overview of the CNMM-DNDC model

110 The CNMM-DNDC is a process-oriented model developed for simulating hydro-biogeochemical interactions at the 111 catchment or site scale, and this model is designed following the basic theories of physics, chemistry, and biogeochemistry 112 and has the capacity to simulate the complex transport and transformation of water, nitrogen and carbon in terrestrial 113 ecosystems under both aerobic and anaerobic conditions. The model can be applied to simultaneously quantify ecosystem productivity, net emissions of nitrogen and carbon gases and hydrological nitrogen losses through soil leaching and 114 115 discharge in streams from an entire catchment or individual landscape unit (Zhang et al., 2018b). The model was established 116 to address the bottleneck issue associated with most biogeochemical models, i.e., the inability to simulate the lateral flows of 117 water and nutrients, by incorporating the core biogeochemical processes of DNDC (including the processes of 118 decomposition, nitrification, denitrification and fermentation) into the hydrological framework of the CNMM, which is fully 119 distributed. For the new generation of biogeochemical models, the microbial ecology was integrated into the biogeochemical 120 models, which represents direct microbial control over decomposition, such as MOMOS (Pansu et al., 2010; Treseder et al., 121 2011; Todd-Brown et al., 2012; Pansu et al., 2014). The biogeochemical processes simulated by the DNDC were generally 122 based on first-order kinetics for decomposition and Michaelis-Menten kinetics of two substrates for nitrification and 123 denitrification, which only the parameterized growth and death of nitrifiers and denitrifiers were considered (Li, 2000). However, due to the global application and validation of DNDC (e.g., Chen et al., 2008; Giltrap et al., 2010; Cui et al., 2014, 124 125 Zhang et al., 2015), the biogeochemical processes of DNDC were selected in the CNMM-DNDC despite some deficiencies 126 in simulating microbial biomass.

127 The simulated soil depth (including bedrock) is user-defined. The temporal and spatial resolutions are also user-128 defined according to the driving data of climate (generally in 3 hours) and digital elevation model (DEM). The soil moisture 129 was calculated based on the mass balance of precipitation, irrigation, evapotranspiration, vertical flow, lateral flow and water 130 from a rising water table. The total water that can be infiltrated during each time step was determined by a defined maximum 131 infiltration rate. Darcy's law was applied for predicting the vertical water flow in the soil profile. A cell-by-cell approach 132 using a kinematic approximation was applied to route the saturated overland and subsurface flow based on DEM. The stream 133 flow was estimated using a cascade of linear channel reservoirs (Wigmosta et al., 1994). For plant growth, gross primary 134 production was simulated using Farquhar et al. (1980) for  $C_3$  and Collatz et al. (1992) for  $C_4$ , with annual primary 135 productivity calculated as the residue of gross primary production and autotrophic respiration. The processes related to the 136 production of N<sub>2</sub>O include nitrification and denitrification, which occur simultaneously at aerobic and anaerobic microsites, 137 respectively. The concept of an "anaerobic balloon" was adopted to determine the microsites and allocate substrates for nitrification and denitrification. The sizes of the aerobic (nitrification) and anaerobic (denitrification) microsites were 138 139 determined by the soil redox potential (Eh) using the Nernst equation (Li, 2007). The "hole in the pipe" concept was applied 140 to calculate N<sub>2</sub>O production during nitrification, which is influenced by the soil moisture, temperature and pH (Li, 2016). 141 The production of N<sub>2</sub>O during denitrification was predicted with Michaelis-Menten kinetics and Pirt functions following the 142 reaction chain of denitrification. The predicted CH<sub>4</sub> flux was influenced by CH<sub>4</sub> production, oxidation and transportation derived from the module of fermentation in the DNDC (Li, 2007). Methane production and oxidation occurred 143 144 simultaneously and were determined by the sizes of the aerobic (production) and anaerobic (oxidation) microsites, which 145 were defined by an Eh calculator in terms of an "anaerobic balloon" ("CH<sub>4</sub> balloon") (Li, 2007). The predicted CH<sub>4</sub> 146 production was calculated from the carbon substrates resulting from decomposed soil organic carbon (SOC) and plant root 147 biomass with the effects of soil temperature (Li, 2000, 2016). For more details, please see Li. (2000, 2007) and Zhang et al. 148 (2018b).

### 149 2.1.2 Modifications of the CNMM-DNDC model

150 In the CNMM-DNDC, the soil temperature was predicted by solving the one-dimensional heat conduction equation 151 with the implicit method of Crank-Nicholson. However, despite the simple parameterization used for the calculation of soil 152 heat capacity and thermal conductivity, the variations of soil temperature induced by the freeze-thaw cycles were also not 153 considered (Table S1 of the online supplementary materials), which inevitably hindered its application in seasonally frozen 154 regions. In this study, the CNMM-DNDC was modified by replacing the above soil thermal module by a physical based 155 module of Northern Ecosystem Soil Temperature (Zhang et al., 2003; Deng et al., 2014), which can explicitly describe the 156 energy exchange within the soil, the active layer dynamics and the soil thermal regime in the presence of freeze-thaw cycles. 157 These modifications are indispensable for accurately simulating freeze-thaw cycles in seasonally frozen regions, which are 158 crucial for characterizing the active layer and soil thermal dynamics, soil hydrology and nitrogen or carbon cycling in these 159 regions. Therefore, the CNMM-DNDC with and without the above modifications are hereafter referred to as the original and 160 modified model, respectively.

161 The modified thermal dynamics of the soil are calculated by the one-dimensional heat conduction equation (Eq. 1). 162 The equation is solved numerically by converting to an explicit form (Eqs. 2–4), which is more efficient for considering the

freeze-thaw cycles (Zhang *et al.*, 2003). In the above equations,  $C (J \text{ m}^{-3} \text{ C}^{-1}), k (W \text{ m}^{-1} \text{ C}^{-1}), T (C)$  and  $G (W \text{ m}^{-2})$  denote 163 164 the soil heat capacity, thermal conductivity, soil temperature and heat fluxes between layers, respectively. Both Z and D are the thicknesses of the soil layer (m),  $\Delta t$  is the time step of the calculation, and l denotes the soil layer l. S is the internal heat 165 exchange due to freezing or thawing (W m<sup>-3</sup>) when the soil temperature is around 0 %. The soil temperature changes 166 affected by freezing or thawing are determined on the basis of energy conservation, which indicate that the latent heat 167 released during freezing equalled the amount of heat required for the increased soil temperature and vice versa. The dynamic 168 soil heat capacity ( $C_h$ , J m<sup>-3</sup>  $C^{-1}$ ) is the weighted average of the heat capacity for five constituents, including organic matter 169  $(C_{l, OM})$ , minerals  $(C_{l, Min})$ , water  $(C_{l, Water})$ , ice  $(C_{l, Ice})$  and air  $(C_{l, Air})$  (Eq. 5). The values of heat capacity for organic matter, 170 minerals, water, ice and air were  $2.5 \times 10^6$ ,  $2.0 \times 10^6$ ,  $4.2 \times 10^6$ ,  $2.1 \times 10^6$  and  $1.2 \times 10^3$  J m<sup>-3</sup> °C<sup>-1</sup>, respectively (Huang, 2000). The 171 weight is the relative volumetric fraction of each constituent ( $\theta_{l, OM}, \theta_{l, Min}, \theta_{l, Water}, \theta_{l, Lee}, \theta_{l, Air}$ ) in the soil. The dynamic 172 thermal conductivity ( $k_l$ , W m<sup>-1</sup>  $C^{-1}$ ) is calculated using the thermal conductivities of above five constituents (Eq. 6–13), 173 with values of 0.25 ( $k_{l, \text{OM}}$ ), 2.9 ( $k_{l, \text{Min}}$ ), 0.57 ( $k_{l, \text{Water}}$ ), 2.2 ( $k_{l, \text{Lee}}$ ) and 0.025 ( $k_{l, \text{Air}}$ ) W m<sup>-1</sup> °C<sup>-1</sup> for organic matter, minerals, 174 175 water, ice and air, respectively (Johansen, 1975). ST<sub>l</sub> denotes the soil temperature of layer l ( $\mathcal{C}$ ). The upper and lower 176 boundary conditions of the thermal dynamics were determined by the surface energy balance and the defined geothermal 177 heat flux at a soil depth of 35 m.

$$C\frac{\partial T}{\partial t} = \frac{\partial}{\partial Z} \left(k\frac{\partial T}{\partial Z}\right) + S \tag{1}$$

$$C_l \frac{\Delta T_l}{\Delta t} = \frac{G_{l-l,l} - G_{l,l+l}}{D_l} + S_l \tag{2}$$

$$G_{l-1,l} = \frac{(0.5k_l + 0.5k_{l-1})(T_{l-1} - T_l)}{0.5D_{l-1} + 0.5D_l}$$
(3)

$$G_{l,l+1} = \frac{(0.5k_l + 0.5k_{l+1})(T_l - T_{l-1})}{0.5D_l + 0.5D_{l+1}}$$
(4)

$$C_{l} = C_{l, \text{ OM}} \theta_{l, \text{ OM}} + C_{l, \text{ Min}} \theta_{l, \text{ Min}} + C_{l, \text{ Water}} \theta_{l, \text{ Water}} + C_{l, \text{ Ice}} \theta_{l, \text{ Ice}} + C_{l, \text{ Air}} \theta_{l, \text{ Air}}$$
(5)

$$k_{l} = \frac{\theta_{l, \text{Water}}k_{l, \text{Water}} + F_{l, \text{Air}}\theta_{l, \text{Air}}k_{l, \text{Air}\_adj} + F_{l, \text{OM+Min}}(\theta_{l, \text{OM}} + \theta_{l, \text{Min}})k_{l, \text{OM+Min}} + F_{l, \text{Ice}}\theta_{l, \text{Ice}}k_{l, \text{Ice}}}{\theta_{l, \text{Water}} + F_{l, \text{Air}}\theta_{l, \text{Air}} + F_{l, \text{OM+Min}}(\theta_{l, \text{OM}} + \theta_{l, \text{Min}}) + F_{l, \text{Ice}}\theta_{l, \text{Ice}}}$$
(6)

$$k_{l, \operatorname{Air}_{adj}} = \begin{cases} k_{l, \operatorname{Air}} + 0.0238e^{0.0536\mathrm{ST}_{l}} & (\theta_{l, \operatorname{Water}} > 0.09) \\ 0.418 \times (0.0615 + 1.96\theta_{l, \operatorname{Water}}) & (\theta_{l, \operatorname{Water}} \ge 0.09) \end{cases}$$
(7)

$$g_a = \begin{cases} 0.333 - \frac{0.298\theta_{l, Air}}{1 - \theta_{l, OM} - \theta_{l, Min}} & (\theta_{l, Water} > 0.09) \\ 0.013 + 0.944\theta_{l, Water} & (\theta_{l, Water} \ge 0.09) \end{cases}$$
(8)

$$g_c = 1.0 - 2.0g_a$$
 (9)

$$k_{l, \text{ OM+Min}} = k_{l, \text{ OM}} \frac{\theta_{l, \text{ OM}}}{\theta_{l, \text{ OM}} + \theta_{l, \text{ Min}}} + k_{l, \text{ Min}} \frac{\theta_{l, \text{ Min}}}{\theta_{l, \text{ OM}} + \theta_{l, \text{ Min}}}$$
(10)

$$F_{l, \operatorname{Air}} = 0.333 \left( \frac{2.0}{1.0 + g_a \left( \frac{k_{l, \operatorname{Air}_a dj}}{k_{l, \operatorname{Water}}} - 1.0 \right)} + \frac{1.0}{1.0 + g_c \left( \frac{k_{l, \operatorname{Air}_a dj}}{k_{l, \operatorname{Water}}} - 1.0 \right)} \right)$$
(11)

$$F_{l, \text{OM+Min}} = 0.333\left(\frac{2.0}{1.0 + 0.125\left(\frac{k_{l, \text{OM+Min}}}{k_{l, \text{Water}}} - 1.0\right)} + \frac{1.0}{1.0 + 0.75\left(\frac{k_{l, \text{OM+Min}}}{k_{l, \text{Water}}} - 1.0\right)}\right)$$
(12)

$$F_{l, \, \text{Ice}} = 0.333 \left( \frac{2.0}{1.0 + 0.125 \left( \frac{k_{l, \, \text{Ice}}}{k_{l, \, \text{Water}}} - 1.0 \right)} + \frac{1.0}{1.0 + 0.75 \left( \frac{k_{l, \, \text{Ice}}}{k_{l, \, \text{Water}}} - 1.0 \right)} \right)$$
(13)

178

Compared to the original thermal module, the internal heat exchange due to freezing or thawing (S) was included with improved algorithm for thermal conductivity (k). In addition, the one-dimensional heat conduction equation (Eq. 1) was solved by converting it to an explicit form in the modified model (Eqs. 2–4), while was solved with the implicit method in the original models (Table S1). The modified CNMM-DNDC was able to simulate the thermal dynamics in seasonally frozen regions as well as their impacts on biogeochemical processes, such as the emissions of nitrogen and carbon gases.

## 184 2.2 Catchment and field descriptions

185 The study area is the Rierlangshan catchment (34°02'N, 102°43'E) on the eastern Tibetan Plateau with an area of 189 186 ha (Yao et al., 2019). This catchment is located in the source region of the Pai-Lung River, which is a sub-branch of the 187 upper Yangtze River (Zhang et al., 2018a; 2019). This region is subject to a cold humid continental monsoon climate, and it 188 had an annual mean air temperature of  $1.6 \pm 0.7$  °C and average annual precipitation of 649 ± 94 mm in 1980–2012 as 189 observed at the Zoige Meteorological Station (~80 km south of the catchment) (Ma et al., 2018). The catchment consists of 190 alpine wetlands, meadows and forests (Yao et al., 2019). The alpine wetlands in the catchment are part of the Zoige wetland 191 and are degraded due to anthropogenic drainage and climate warming (Dong et al., 2010; Li et al., 2014). Degraded alpine 192 wetlands are commonly distributed throughout the Zoige wetland, and nearly 83% of the permanently inundated wetlands 193 have been converted into "wet grassland" (Xiang et al., 2009; Li et al., 2014).

194 CH<sub>4</sub> and N<sub>2</sub>O fluxes were manually measured once or twice per week using the gas chromatograph-based static opaque 195 chamber method (Zhang et al., 2018a) at three sites in alpine wetlands (34°02'6.53"N, 102°43'29.66"E, 3304 m a.s.l.), 196 meadows (34°02'01"N, 102°43'28"E, 3326 m a.s.l.) and forests (34 °01'47.13"N, 102°44'0.87"E, 3415 m a.s.l.) in the 197 Rierlangshan catchment from 2013 to 2015 (Zhang et al., 2018a; Yao et al., 2019; Zhang et al., 2019) (Fig. S1). Each 198 chamber was wrapped with a layer of styrofoam and aluminium foil to mitigate temperature increases inside the enclosures 199 due to the heating of solar radiation. The alpine wetland site is located at a slope base with a slope of 2°. The wetland has 200 suffered from anthropogenic drainage and climate warming, and thus degraded to be seasonally inundated. The alpine 201 meadow site neighbours the alpine wetland site, which is located on the north-facing slope with gradient of 11°. In addition, 202 soil temperatures at different depths and topsoil moisture in the alpine wetlands, meadows and forests were observed daily and twice per week, respectively. The details regarding the available field observations of the  $CH_4$  and  $N_2O$  fluxes and the relevant auxiliary variables are described in Table S2.

#### 205 2.3 Model simulation

206 The modified CNMM-DNDC was applied in the Rierlangshan catchment with the three alpine ecosystems; wetlands, 207 meadows and forests. The dataset required for the catchment simulation included (1) a digital elevation model (DEM) with a resolution of  $30 \times 30$  m<sup>2</sup> from the geospatial data cloud (Fig. S1; http://www.gscloud.cn/); (2) a map of alpine ecosystems, 208 including wetlands, meadows and forests; (3) a climate dataset of 3-hour weather data (air temperature, precipitation, wind 209 210 speed, solar radiation, longwave radiation, and humidity), which were obtained from the meteorological station in the target 211 catchment for the years with field observations (2013.11-2015.10) and were adapted from the daily data at the Zoige Meteorological Station (provided by the National Meteorological Information Center: http://data.cma.cn/: last access: 10<sup>th</sup> 212 213 June, 2020) for other years; (4) a soil properties dataset of the observed clay fraction, organic matter content, total nitrogen, 214 pH and bulk density of the three alpine ecosystems in 1 m soil profile (Ma et al., 2018; Zhang et al., 2018a; Yao et al., 2019; 215 Zhang et al., 2019; Table S3); and (5) a management practices dataset including grazing time and intensity for the alpine 216 wetlands and meadows (Table S3). In addition, other required soil inputs of field capacity, wilting point and saturated 217 hydrological conductivity were calculated by pedo-transfer functions (Li et al., 2019; Table S4). The simulated soil depth 218 was defined as 35 m due to the lower boundary conditions of the thermal dynamics, which was set as the geothermal heat 219 flux at a soil depth of 35 m. The simulated soil profile (0-35 m depth) was divided into 23 layers, including the soil (0-1.5220 m) and bedrock (1.5-35 m). The layer thicknesses of the soil (0-1.5 m) were 0.01, 0.05, 0.1 and 0.5 cm for the depth of 0-221 0.1, 0.1–0.2, 0.2–1 and 1–1.5 m, respectively. The layer thicknesses of the bedrock (1.5–35 m) were 3.5 and 31m for the depth of 1.5–4.0 and 4.0–35 m, respectively. The geothermal heat flux in the catchment was estimated at 0.053 W m<sup>-2</sup> 222 223 (Pollack and Chapman, 1977). For the target catchment, the soil water dynamics of the alpine ecosystems were determined 224 by the precipitation, evapotranspiration, infiltration, penetration and lateral flow. Using the database, a catchment simulation of hydro-biogeochemical processes was performed with spatial and temporal resolutions of  $30 \times 30$  m<sup>2</sup> and 3 hours, 225 226 respectively, by the modified CNMM-DNDC from 2012 to 2015, which could reflect the influences of hydrological 227 processes on soil water dynamics. Thus, the soil water dynamics of the seasonally inundated wetlands were determined by 228 the hydrological processes without any artificial disturbances in the catchment simulation.

#### 229 2.4 Statistics and analysis

The statistical criteria applied for evaluating the model performance in this study included (i) the index of agreement (IA), (ii) the Nash–Sutcliffe efficiency (NSE), and (iii) the determination coefficient ( $R^2$ ) and slope of the zero-intercept univariate linear regression (ZIR) of the observations against the simulations (e.g., Nash and Sutcliffe, 1970; Willmott and Matsuura, 2005; Moriasi *et al.*, 2007; Congreves *et al.*, 2016; Jiang, 2010; Dubache *et al.*, 2019). A value of IA (0–1) closer to 1 showed a better simulation. An NSE value (ranging from minus infinity to 1) closer to 1 was better. Better model 235 performance was indicated by a slope and an  $R^2$  value that were both closer to 1 in a significant ZIR. The significance level

236 of the ZIR was indicated by the P value. For more details on these criteria, refer to the Eqs. S1-4 in Table S5. In addition,

the SPSS Statistics Client 19.0 (SPSS Inc., Chicago, USA) and Origin 8.0 (OriginLab, Northampton, MA, USA) software

238 packages were applied for the statistical analysis and graphical comparison.

## 239 3 Results

# 240 3.1 Model validation

# 241 3.1.1 Soil temperature and moisture

242 The profile soil temperatures were observed for alpine wetland and meadow, but only topsoil temperature was 243 observed for the alpine forest, which could be used for model validation. The simulated soil temperatures of the three typical 244 alpine ecosystems were significantly improved by including the scientific processes of soil thermal dynamics suitable for seasonally frozen regions (Figs. 1 and S2). The simulated seasonal dynamics and magnitudes were consistent with those 245 from the field observations for various soil depths, with IA, NSE, and ZIR slopes and  $R^2$  values of 0.91–1.00, 0.68–0.99, 246 247 0.83-1.09 and 0.73-1.00 for the three alpine ecosystems, respectively (Table 1). For the observed alpine wetlands and meadows, the simulation showed that the freezing of soil started in early November and continued to the end of April in the 248 249 next year. The frozen depth reached a maximum in the middle of February. However, the simulated maximum frozen depths for the observed alpine meadows (0.69–0.74 m) were approximately double those for the alpine wetlands (0.30–0.39 m) (Fig. 250 S3). 251

252 For the soil moisture, only topsoil moisture was observed in the three alpine ecosystems, which could be applied for 253 model validation. The simulated topsoil moisture dynamics were comparable to those from the field observations, with IA 254 and NSE values of 0.49-0.83 and -0.80-0.32 for the three alpine ecosystems, respectively (Fig. 2 and Table 1). In 255 comparison to the other alpine ecosystems, the alpine wetlands had higher soil moisture, which ranged from 0.41 to 0.98 and 256 from 0.38 to 0.93 for the observations and simulations in the water-filled pore space (WFPS), respectively. The soil moisture 257 values of the alpine meadows and forests were highly variable and depended on the variation trend in precipitation for both 258 observations and simulations. However, an underestimation of soil moisture in the winter period occurred for both alpine 259 meadows and forests due to a possible overestimation of evapotranspiration. The performances of the modified model in 260 simulating the soil profile temperature and topsoil moisture indicate that the modified CNMM-DNDC can generally predict the soil thermal and topsoil moisture dynamics in the three alpine ecosystems, which is crucial for correctly simulating soil 261 262 hydrology, plant growth and biogeochemical processes.

#### 263 3.1.2 Methane fluxes

264 The daily observed  $CH_4$  emissions from the alpine wetlands were highly variable and showed a clear seasonal cycle, 265 with intensive  $CH_4$  emissions from May to November and weak emissions in other periods (Fig. 3a). The observed alpine 266 meadows and forests functioned exclusively as sinks of atmospheric  $CH_4$  with higher rates of uptake during the growing season and lower uptake rates in the dormant season (Figs. 3b-c). The original model significantly overestimated CH<sub>4</sub> 267 268 emissions from the alpine wetlands. The modified CNMM-DNDC accurately identified the functions of the sources or sinks in the three alpine ecosystems and generally captured the magnitude and seasonal characteristics of the daily  $CH_4$  fluxes, 269 270 with an IA of 0.57-0.88 for the three alpine ecosystems (Figs. 3a-c and Table 1). However, the CH<sub>4</sub> uptake rates during the 271 dormant season were obviously underestimated by the modified model at both sites, especially at the alpine forest site, which 272 was responsible for the underestimation of cumulative  $CH_4$  uptake. The observed cumulative  $CH_4$  emissions ranged from -2.60 to 33.5 kg C ha<sup>-1</sup> vr<sup>-1</sup> and the modelled values ranged from -1.90 to 31.0 kg C ha<sup>-1</sup> vr<sup>-1</sup> (Fig. 4a). These results indicate 273 274 that the modified CNMM-DNDC well simulated the  $CH_4$  fluxes of the three typical alpine ecosystems.

#### 275 3.1.3 Nitrous oxide fluxes

276 The daily observed  $N_2O$  emissions from the alpine wetlands were higher than those from the alpine meadows but 277 lower than those from the alpine forests (Figs. 3d-f). Similar seasonal patterns of N<sub>2</sub>O fluxes were observed for the three 278 alpine ecosystems with intensive emissions in the growing season. The  $N_2O$  emission peak during the dormant season was 279 observed in the alpine meadows, which was the major contributor to annual emissions. The modified CNMM-DNDC 280 generally captured the seasonal dynamics of daily  $N_2O$  fluxes with an IA of 0.26–0.47 for the three alpine ecosystems (Figs. 3d-f and Table 1), but the N<sub>2</sub>O emissions from the alpine wetlands were significantly overestimated by the original model. 281 282 For the modified model, the simulated N<sub>2</sub>O emissions from the alpine wetlands and forests showed obvious seasonal patterns 283 with higher emissions during the growing season, but no abrupt emission peak was captured at the end of the growing season 284 for the alpine wetlands. In addition, compared with the original model, the modified model captured the peak emissions that occurred during the freeze-thaw period from the alpine meadows due to the death of microbes, but the dynamics of the peak 285 emissions were not well simulated. The observed cumulative N<sub>2</sub>O emissions ranged from 0.14 to 0.58 kg N ha<sup>-1</sup> yr<sup>-1</sup> and the 286 modelled values ranged from 0.12 to 0.32 kg N ha<sup>-1</sup> yr<sup>-1</sup> (Fig. 4b). These results indicate that the modified CNMM-DNDC 287 288 has the potential to estimate N<sub>2</sub>O emissions in seasonally frozen regions.

## 289 3.2 Annual aggregate emissions of CH<sub>4</sub> and N<sub>2</sub>O

Annual aggregate emissions of  $CH_4$  and  $N_2O$  in carbon dioxide ( $CO_2$ ) equivalents were calculated for the three alpine ecosystems from November 2013 to November 2014 for alpine wetlands and meadow and from April 2014 to April 2015 for alpine forests, and the global warming potentials were 34 for  $CH_4$  and 298 for  $N_2O$  on a 100-year time horizon (IPCC, 2013). The simulated aggregate emissions by the modified model were 1.5, 0.015, and 0.061 Mg  $CO_2$ eq ha<sup>-1</sup> yr<sup>-1</sup> for the observed alpine wetlands, meadows and forests, respectively, which were consistent with those from the field observations (1.6, 0.014, and 0.15 Mg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> for the alpine wetlands, meadows and forests, respectively) (Fig. 4c). However, the original model significantly overestimated the aggregate emissions due to the high predicted CH<sub>4</sub> and N<sub>2</sub>O emissions. In comparison, the observed seasonally inundated wetlands functioned as the sources of aggregate emissions of CH<sub>4</sub> and N<sub>2</sub>O, but the aggregate emissions from adjacent wet alpine meadows were much lower.

#### 299 4 Discussions

#### **300 4.1 Model performance in simulating thermal dynamics**

301 The soil freeze-thaw cycles in seasonally frozen regions determine the soil profile temperature and hydrological 302 processes, which are key factors that regulate the cycling of nitrogen and carbon (e.g., Zhang et al., 2015; Hugelius et al., 303 2020). Therefore, improving the scientific processes of soil thermal dynamics in the presence of active layer dynamics is 304 essential for applying the CNMM-DNDC to simulate the biogeochemical processes in seasonally frozen regions, which are 305 sensitive and vulnerable to climate change and human activities (Hatano, 2019; Hugelius et al., 2020; Jiang et al., 2020). The 306 original model adopted a relatively simple module to calculate thermal transportation within the soil profile and did not 307 consider the effects of freeze-thaw cycles on soil temperature and moisture. The newly incorporated module was based on 308 explicit energy conservation and exchange in the soil profile and successfully captured the variations in soil temperature and 309 topsoil moisture for the three alpine ecosystems during the freeze-thaw period. The simulated lower soil frozen depth for the 310 observed alpine wetland was primarily attributed to the higher soil profile moisture level, as the thermal conductivity and 311 heat capacity for water-filled pores were higher than those for air-filled pores. In order to quantify the impacts of climate 312 change on the cycling of carbon and water on the regional and global scales, several large scale ecosystem models or 313 macroscale hydrological models, such as Terrestrial Ecosystem Model, Lund-Potsdam-Jena dynamic global vegetation 314 model and Variable Infiltration Capacity model, have been enhanced to simulate the soil thermal dynamics at northern high 315 latitude (e.g., Wania et al., 2009; Zhuang et al., 2001; Cuo et al., 2015; Jiang et al., 2020). In addition, the soil thermal 316 modules were also improved in some biogeochemical models, such as DNDC and Mobile-DNDC, to evaluate the influences 317 of climate warming on the biogeochemical processes in high latitude regions (e.g., Zhang et al., 2003; de Bruijn et al., 2009; 318 Wolf et al., 2011; Zhang et al., 2012; Deng et al., 2014). Compared with the simulated soil profile temperatures by above 319 models at different scales, the simulations in this study by the modified CNMM-DNDC were equally well, especially for 320 deeper soil layers (e.g., Wania et al., 2009). For the validated topsoil moisture in this study, the modified model generally 321 captured the variation trends, which were comparable with the performances of other models (e.g., de Bruijn et al., 2009; 322 Wolf et al., 2011; Cuo et al., 2015). However, compared with the studies focused on simulating soil moisture (e.g., Ford et 323 al., 2014), further improvements are still required to improve the model performance in simulating the soil moisture. These 324 results indicate the efficiency of the incorporated module in simulating soil thermal and topsoil moisture dynamics in 325 seasonally frozen regions.

#### 326 4.2 Model performance in simulating CH<sub>4</sub> fluxes

327 Compared with the annually inundated wetlands, the seasonally inundated wetlands had relatively low observed and 328 simulated  $CH_4$  emissions due to the significant influences of the water table level on  $CH_4$  emissions (e.g., Hatano, 2019; 329 Zhang et al., 2019). The CH<sub>4</sub> emissions simulated by the CNMM-DNDC were determined by the processes of production, 330 oxidation and transpiration. The unsaturated soil with moisture levels ranging from 0.41 to 0.98 WFPS resulted in a small 331  $CH_4$  balloon and thus reduced  $CH_4$  production. At the same time, relatively dry conditions caused the upper soil layer to act 332 as an efficient oxidative methanotrophic barrier for the diffusion of  $CH_4$  from the subsoil and thus decreased  $CH_4$  emissions 333 (Kandel et al., 2018; Tan et al., 2020). In addition, the highly fluctuating CH<sub>4</sub> emissions simulated by the modified model 334 were also attributed to the high dependency of  $CH_4$  production on soil moisture, which controlled the size of the  $CH_4$  balloon. 335 Theoretically, the  $CH_4$  emissions simulated by the original model should not be higher than those simulated by the modified 336 model due to the lower predicted soil moisture level. The overestimated  $CH_4$  emissions simulated by the original model were 337 mainly attributed to the overestimated soil temperature due to their influences on mineralized substrates for CH<sub>4</sub> production, 338 as well as the processes of  $CH_4$  production. This result implies that global warming may trigger intensive  $CH_4$  emissions 339 from degraded wetlands, which could partly serve as a trade-off for the decreased  $CH_4$  emissions due to the lower water table 340 level in degraded wetlands (e.g., Gong *et al.*, 2020). For the studies focused on simulating  $CH_4$  emissions from wetlands by 341 the large-scale ecosystem models, the model validation with field observation is difficult due to coarse spatial resolution (e.g., 342 Zhuang et al., 2004). For the biogeochemical model, such as DNDC, the dynamics of CH<sub>4</sub> emissions from wetland and peatland in the northern permafrost regions were well simulated (Zhang et al., 2012; Deng et al., 2014), which showed 343 344 consistent seasonal variations and magnitudes as those in this study. Both observations and simulations showed that the  $CH_4$ 345 uptake in alpine forests was higher than that in alpine meadows, which was mainly attributed to the high SOC content of the 346 alpine forests in the simulation. Methane uptake by upland soils is a biological process governed by the availability of  $CH_4$ 347 and oxygen as well as the activity and quantity of methanotrophic bacteria in soils (e.g., Liu et al., 2007; Zhang et al., 2014). 348 In the model, the simulated  $CH_4$  uptake was positively related to the SOC content, which is closely related to the population 349 size of methanotrophic bacteria. Thus, the SOC content primarily contributed to the differences in  $CH_4$  uptake from alpine 350 meadows and forests, as the values for forests were more than twice of those for meadows (Table S3). As the simulated 351 dynamic characteristics of CH<sub>4</sub> uptake were primarily regulated by soil temperature and moisture, the inhibitory effects of 352 low soil temperature (< 0.0  $^{\circ}$ C) on CH<sub>4</sub> uptake rates resulted in obvious underestimations in the dormant season for both 353 alpine meadows and forests. Therefore, an improved parameterization for simulating  $CH_4$  uptake under low soil temperatures 354 is required for the model to better capture the dynamics of CH<sub>4</sub> uptake in the dormant season.

#### 355 4.3 Model performance in simulating N<sub>2</sub>O fluxes

In comparison, the  $N_2O$  emissions from the alpine wetlands and forests were higher than those from the alpine meadows for both the observations and simulations due to the high SOC content and nitrogen availability. Natural wetlands 358 are large carbon reserves and play a crucial role in mitigating global warming (e.g., Deng et al., 2014; Kang et al., 2020; Tan 359 et al., 2020). The intentional drainage of annually inundated wetlands alters not only the water regime but also nutrient 360 availability (e.g., Hoffmann et al., 2016). The simulated relatively low soil moisture for the alpine wetlands stimulated the 361 decomposition of SOC and nitrogen (or peat oxidation) under aerobic conditions, thus improving nitrogen mineralization for 362 nitrification and denitrification and enhancing N<sub>2</sub>O emissions (e.g., Tan *et al.*, 2020; Zhang *et al.*, 2020). The intensive N<sub>2</sub>O 363 emissions simulated by the original model resulted from the overestimated soil temperature for the alpine wetlands. Firstly, 364 as the presence of ice could impede the water movement, the water lateral flows were promoted by the original model due to 365 the neglecting of freeze-thaw cycles. These further resulted in the lower simulated soil moisture as compared with the modified model (Fig. S4), which provided favorable oxygen conditions for  $N_2O$  production. Meanwhile, the simulated high 366 soil moisture by the modified model provided feasible anaerobic conditions for thoroughly denitrification. Secondly, higher 367 368 simulated soil temperature by the original model also facilitated the mineralization, which provided more available mineral 369 nitrogen. Field studies showed that high SOC concentrations could stimulate the processes of mineralization and nitrification 370 in the forests (e.g., Li et al., 2005; Yao et al., 2019). The model input of soil organic matter measured in the observed alpine 371 forests was more than twice that in the observed alpine meadows (Table S3). Thus, the high SOC content at the alpine forest 372 site provided more available nitrogen through mineralization and thus stimulated the nitrification processes in the simulation. 373 Furthermore, the seasonal grazing that occurred in the alpine meadows resulted in constant loss of available nitrogen and 374 thus hindered the N<sub>2</sub>O emissions from the biological processes in the simulation. Field observations showed that the soil 375 freeze-thaw cycles occurred in seasonally frozen regions not only increased the availability of nitrogen and carbon substrates 376 by disrupting of soil aggregates but also affected the structure, population and activity of the microbes, and thus influencing 377 the emissions of N<sub>2</sub>O (e.g., Song et al., 2019). de Bruijn et al. (2009) have explored the combined mechanisms for 378 simulating freeze-thaw related N<sub>2</sub>O emissions, which were the promoted anaerobiosis and denitrification due to reduced gas 379 diffusion derived from soil frost and snow cover, and the stimulated microbial growth due to easy decomposable organic 380 carbon and nitrogen derived from the dead microbes during freeze-thaw cycles. Wolf et al. (2011) introduced an impedance 381 factor to parameterize the reduced water flow between layers in the presence of ice, which could captured the freeze-thaw 382 related  $N_2O$  emissions for ungrazed steppe. In the CNMM-DNDC, threshold values of soil temperature were set to trigger 383 the death of microbes during the freezing period and stimulate the production of NO, N<sub>2</sub>O and N<sub>2</sub> using substrates derived 384 from the dead microbes during the thawing period, which was similar to one of the mechanisms explored by de Bruijn et al. 385 (2009). However, compared with the simulated freeze-thaw related  $N_2O$  emissions by other studies, the simulated dynamics 386 of peak emissions due to freeze-thaw cycles in this study were inconsistent with those from the field observations. Thus, 387 improvements are required to incorporate some other effective mechanisms to better capture the dynamic characteristics. The 388 peak emissions during the freeze-thaw period were not captured by the original model due to the significantly overestimated 389 soil temperature. The low evaluation statistics for the daily fluxes, especially for the alpine forests, were also attributed to the 390 underestimation of background emissions, which resulted from both measurement errors due to low fluxes around detection limits ( $\pm 0.41$  g N ha<sup>-1</sup> d<sup>-1</sup>) and model deficiencies in the simulation of tight nitrogen cycling in natural ecosystems. 391

392 Compared with the empirical model, one key advantage of the process-oriented models is that the models are 393 independent of the local parameterization (Zhang et al., 2015). In this study, default internal parameter combinations of 394 biogeochemical processes were used for the original and modified models, which have been applied in the catchment 395 simulation in the subtropical region (Zhang et al., 2018b), due to the limited field observations (only one year) for both 396 calibration and validation. The biogeochemical processes were predicted by the first-order and Michaelis-Menten kinetics in 397 the CNMM-DNDC based on some defined parameters of flow fractionation. For instance, there are 17 parameters related 398 with  $N_2O$  emission in the module of denitrification (Table S6), which would inevitably increase the uncertainty of simulation. 399 Houska et al. (2017) found that hydro-biogeochemical models can be right for the wrong reasons, such as matching 400 greenhouse gas emissions while failing to simulate soil moisture, which emphasized the importance for simultaneous 401 validations of multi-variables. Thus, simultaneous validations of CH<sub>4</sub> and N<sub>2</sub>O fluxes, as well as soil environment variables, 402 were necessary for comprehensive evaluation of the model performance. In addition, the microbial ecology was recently 403 recommended to be integrated into the biogeochemical model using a smaller number of well-defined kinetic parameters, 404 such as MOMOS (Pansu et al., 2010; Treseder et al., 2011). Therefore, direct control of microbial on biogeochemical 405 processes, such as the stoichiometry of decomposer, is required to be included in the CNMM-DNDC in near future. The 406 model performances of simulating various variables for three typical alpine ecosystems in the Rierlangshan catchment imply that the modified CNMM-DNDC can be applied to predict the thermal dynamics and fluxes of CH<sub>4</sub> and N<sub>2</sub>O from alpine 407 408 ecosystems in seasonally frozen regions.

#### 409 **5 Conclusions**

410 To apply the process-oriented hydro-biogeochemical model Catchment Nutrient Management Model - DeNitrification-411 DeComposition (CNMM-DNDC) in seasonally frozen regions, an improved module of soil thermal dynamics for describing 412 the soil thermal regime in the presence of freeze-thaw cycles was incorporated in this study. Using the unique experimental dataset obtained in the Rierlangshan catchment with the typical alpine wetland, meadow and forest ecosystems, the modified 413 model was evaluated for simulating soil thermal dynamics (soil profile temperature), topsoil moisture and fluxes of methane 414 415  $(CH_4)$  and nitrous oxide  $(N_2O)$  in seasonally frozen regions of the Tibetan Plateau. The modified CNMM-DNDC could 416 generally capture the seasonal dynamics and magnitudes of profile soil temperature, topsoil moisture and fluxes of  $CH_4$  and N<sub>2</sub>O in seasonally frozen regions. Both the observed and simulated CH<sub>4</sub> and N<sub>2</sub>O fluxes from three alpine ecosystems 417 indicate that the aggregate emissions of  $CH_4$  and  $N_2O$  were highest for the wetland among three alpine ecosystems. The 418 419 intensive aggregate emissions of  $CH_4$  and  $N_2O$  were regulated by the high soil moisture, which was primarily determined by 420 the CH<sub>4</sub> emissions. This study implies that a hydro-biogeochemical model, such as the modified CNMM-DNDC, are able to 421 predict soil thermal dynamics, topsoil moisture and fluxes of  $CH_4$  and  $N_2O$  in seasonally frozen regions with an improved 422 physical-based soil thermal module.

## 423 Data availability

- 424 The model, input, output and code can be obtained from http://doi.org/10.6084/m9.figshare.14685441. All the observed data
- 425 sets used in this study can be available from the co-authors.

#### 426 Author contribution

427 Zheng, X. and Zhang, W. contributed to developing the idea and enhancing the science of this study. Zhang, W. improved 428 the scientific processes of the model, implemented the model simulations and prepared the manuscript with contributions 429 from all co-authors. Li, S. improved the model structure for standard input. Yao, Z., Zhang, H., Ma, L., Wang, K., Wang, R. 430 and Liu, C. designed and carried out the field experiments. Han, S. collected and established the input database for modelling. 431 Deng, J and Li, Y contributed to the modification of the model and the improvement of the manuscript.

#### 432 Competing interests

433 The authors declare that they have no conflict of interest.

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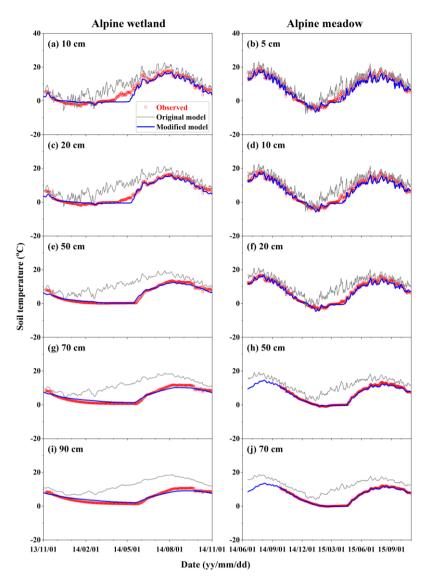
Table 1 Statistics of the validated variables by the modified CNMM-DNDC for three typical alpine ecosystems.

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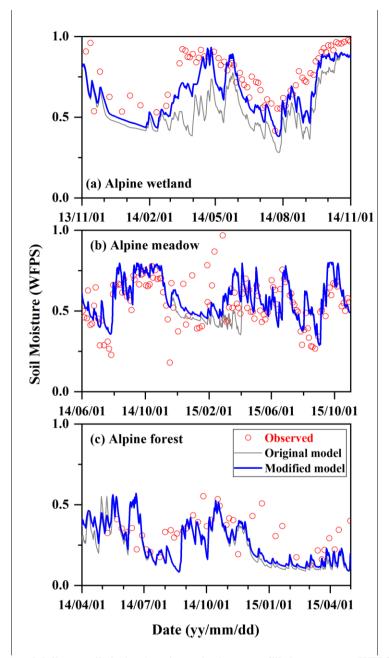
Item	Ecosystem	n <sup>a</sup>	DR⁵	IA		NSE		ZIR-slope		ZIR- $R^{2e}$		ZIR-P	
	-			O <sup>c</sup>	$M^d$	0	М	Ο	М	0	М	0	М
Soil temperature													
5 cm	Meadow	500	Daily	0.90	0.96	0.82	0.95	0.84	1.09	0.89	0.96	< 0.001	< 0.001
	Forest	48	Daily	0.85	0.91	0.37	0.68	0.64	0.83	0.68	0.73	< 0.001	< 0.001
10 cm	Wetland	366	Daily	0.90	0.98	0.57	0.92	0.72	1.07	0.81	0.93	< 0.001	< 0.001
	Meadow	500	Daily	0.93	0.99	0.71	0.95	0.80	1.08	0.85	0.96	< 0.001	< 0.001
20 cm	Wetland	366	Daily	0.82	0.99	0.18	0.96	0.64	1.05	0.66	0.97	< 0.001	< 0.001
	Meadow	500	Daily	0.87	0.99	0.48	0.97	0.74	1.06	0.76	0.98	< 0.001	< 0.001
50 cm	Wetland	366	Daily	0.66	0.99	-1.01	0.97	0.51	1.05	0.43	0.97	< 0.001	< 0.001
	Meadow	401	Daily	0.70	1.00	-0.48	0.99	0.58	1.06	0.53	1.00	< 0.001	< 0.001
70 cm	Wetland	366	Daily	0.58	0.98	-2.23	0.93	0.47	1.05	0.38	0.93	< 0.001	< 0.001
	Meadow	401	Daily	0.64	1.00	-1.19	0.99	0.54	1.03	0.49	1.00	< 0.001	< 0.001
90 cm	Wetland	366	Daily	0.52	0.98	-4.07	0.90	0.44	1.03	0.36	0.90	< 0.001	< 0.001
Soil moisture	Wetland	74	Daily	0.63	0.83	-1.65	0.20	1.31	1.13	_	0.60	_	< 0.001
	Meadow	128	Daily	0.78	0.78	0.28	0.32	0.96	0.93	0.30	0.41	< 0.001	< 0.001
	Forest	40	Daily	0.48	0.49	-1.04	-0.80	1.21	1.19	_	_	_	_
Daily CH <sub>4</sub> flux	Wetland	180	Daily	0.37	0.74	-11.1	-0.73	0.46	0.87	_	_	_	_
	Meadow	168	Daily	0.87	0.88	0.42	0.38	1.09	0.94	0.44	0.39	< 0.001	< 0.001
	Forest	49	Daily	0.59	0.57	-2.79	-3.39	0.92	0.79	_	_	_	_
DailyN <sub>2</sub> O flux	Wetland	180	Daily	0.01	0.26	-323	-0.07	0.01	0.59	_	_	_	_
	Meadow	168	Daily	0.23	0.44	-0.16	-1.76	0.99	0.35	_	_	_	_
	Forest	58	Daily	0.47	0.47	-1.85	-1.64	0.44	0.47	_	_	_	_

 $a^{a}$  *n* indicates the number of the observations. <sup>b</sup> DR denotes the time resolution of the observed data. <sup>c</sup> O indicates the simulations by the original model. <sup>d</sup> M indicates the simulations by the modified model. <sup>e</sup> "–" indicated no value due to the sum of regression square are larger than the sum of the total square for the regression). IA, NSE, ZIR-slope, ZIR- $R^{2}$  and ZIR-P indicate the index of agreement, Nash–Sutcliffe efficiency, determination coefficient and slope of the zero-intercept univariate linear regression (ZIR) of the observations against the simulations, as well as

660 the significance level of the ZIR.



661 662 Figure: 1 Observed and simulated daily profile soil temperature from the alpine wetlands and meadows by the original and 663 modified models. The legends in panel a apply for all panels.



664 665 Figure: 2 Observed and simulated daily topsoil (0-6 cm) moisture in the water-filled pore space (WFPS) from the alpine wetlands, 666 meadows and forests by the original and modified models. The legends in panel a apply for all panels.

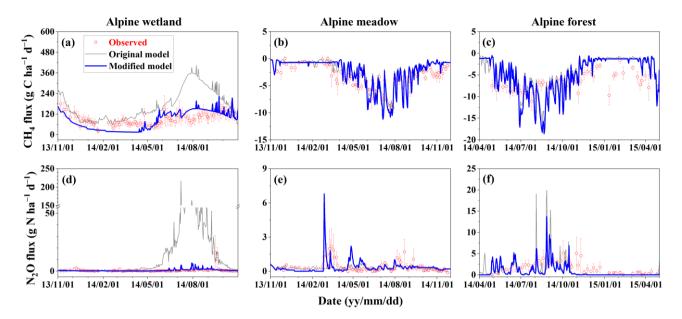
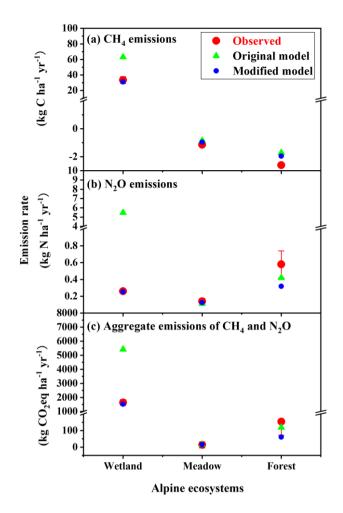
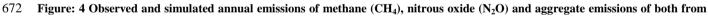




Figure: 3 Observed and simulated daily methane (CH<sub>4</sub>) and nitrous oxide (N<sub>2</sub>O) fluxes from the alpine wetlands, meadows and forests by the original and modified models. The vertical bar for each observation indicates the standard error of six spatial replicates. The legends in panel a apply for all panels.





673 the alpine wetlands (Wetland), meadows (Meadow) and forests (Forest). The legends in panel a apply for all panels.