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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

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Abstract. To evaluate the sustainability of terrestrial ecosystems, the hydro-biogeochemical model Catchment Nutrient Management Model - DeNitrification-DeComposition (CNMM-DNDC) was established to simultaneously quantify ecosystem productivity and losses of nitrogen and carbon at the site or catchment scale. As a process-oriented model, this model is expected to be universally applied to different climate zones, soils, land uses and field management practices. This study, as one of many efforts to fulfil such an expectation, was performed to improve the CNMM-DNDC by incorporating a physical-based soil thermal module to simulate the soil thermal regime in the presence of freeze-thaw cycles. The modified model was validated with simultaneous field observations in three typical alpine ecosystems (wetlands, meadows and forests) within a catchment located in the seasonally frozen region of the eastern Tibetan Plateau. Then, the model was further applied to evaluate its performance in simulating the effects of alpine wetland degradation on methane (CH_4) and nitrous oxide (N_2O) fluxes. The validation showed that the modified CNMM-DNDC was able to simulate the observed seasonal dynamics of soil temperature, moisture, and fluxes of CH_4 and N_2O in the three typical alpine ecosystems, with index of agreement values 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 observations, the simulated aggregate emissions of CH_4 and N_2O were significantly reduced due to wetland degradation and were dominated by a reduction in CH_4 emissions. This study indicates the potential for utilizing the process-oriented model CNMM-DNDC to predict hydro-biogeochemical processes, as well as related gas emissions, in seasonally frozen regions. As the original CNMM-DNDC was previously validated in some unfrozen regions, the modified CNMM-

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DNDC could be applied to evaluate the sustainability of various ecosystems under different climates, soils and field management practices at the site or catchment scale.

1 Introduction

The elements of nitrogen and carbon are essential components of ecosystems (e.g., Breuer *et al.*, 2010; Canfield *et al.*, 2010). Climate changes due to warming and human anthropogenic activities derived from food production have significantly altered the cycling of nitrogen and carbon and led to increased reactive nitrogen availability and carbon losses, which result in a series of environmental problems at the catchment, regional and even global scales (e.g., Galloway *et al.*, 2004; Galloway *et al.*, 2008; Ju *et al.*, 2009). Excessive reactive nitrogen in soils can be lost in the forms of nitrogen gases, such as nitrous oxide (N_2O), nitric oxide (NO) and ammonia (NH_3), and nitrogen pollution, such as nitrate (NO_3^-) and ammonium (NH_4^+), in water through leaching or surface runoff (e.g., Seitzinger, 2008; Collins *et al.*, 2016). In the face of increased air temperatures and intensive land use changes, especially in cold regions, the soil organic carbon stored during long periods has been lost to the atmosphere via methane (CH_4) and carbon dioxide (CO_2) (e.g., Piao *et al.*, 2009; Fenner and Freeman, 2011; Schuur *et al.*, 2015). These nitrogen and carbon losses contribute to potential global warming (CO_2, CH_4 and N_2O), air pollution (NO and NH_3) and surface/groundwater pollution (NO_3^- and NH_4^+). Therefore, sustainable ecosystems urgently need to be established that not only focus on net primary productivity but also are friendly to the environment with the minimal hazards, including greenhouse gases, air pollution and water pollutants (e.g., Cui *et al.*, 2018; Zhang *et al.*, 2019).

The cycling of nitrogen and carbon is closely related to soil water processes (e.g., Breuer *et al.*, 2010; Vereecken *et al.*, 2016; Zhang *et al.*, 2018). Thus, interactions among soil waters and the cycling of nitrogen and carbon govern biological productivity and environmental outcomes (e.g., Zhu *et al.*, 2018). The interactions consist of the redox potential for different transformation processes influenced by the spatiotemporal variation in soil water content and the lateral transport of water and dissolved nitrogen or carbon controlled by surface and subsurface flow (e.g., McClain *et al.*, 2003; Castellano *et al.*, 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., Zhu *et al.*, 2012; Keiluweit *et al.*, 2017). Therefore, a complete understanding of biogeochemical processes will inevitably involve interactions among soil water and the cycling of nitrogen and carbon (e.g., Breuer *et al.*, 2010; Vereecken *et al.*, 2016; Zhu *et al.*, 2018).

Biogeochemical models, such DNDC, WNMM, CENTURY and DayCent, are effective tools for simulating the cycling of nitrogen and carbon and quantifying the effects of climate change and human anthropogenic activities on ecosystems (e.g., Foereid *et al.*, 2007; Li, 2007; Li *et al.*, 2007; Cheng *et al.*, 2014). However, comprehensive hydrological processes, especially for the lateral transport of water and nutrients, are generally simplified or ignored in these models due to specific questions that must be addressed (e.g., Li, 2007; Li *et al.*, 2007; Chen *et al.*, 2008; Deng *et al.*, 2014). On the other hand, land surface or hydrological models at large scales, which are designed with explicit mechanisms of hydrology,

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generally focus on vertical and lateral nutrient transport, such as nitrate loads into rivers (e.g., Liu *et al.*, 2019). However, the simulations of nitrogen and carbon processes are usually based on empirical functions even without predicting gas loss. Due to the various purposes of different models, coupling soil hydrological models with biogeochemical models can be an effective strategy for integrating soil water and cycling of nitrogen and carbon to improve model performance. Thus, the coupled model with improved performance can be applied to evaluate the sustainability of natural or agricultural ecosystems, simultaneously predicting productivity and potential negative environmental effects (e.g., Zhang *et al.*, 2018; Zhu *et al.*, 2018).

In recent years, efforts have been implemented to couple models, such as SWAT-N, LandscapeDNDC-CMF, APSIM, SWAT-DayCent, and CNMM-DNDC (e.g., Pohlert *et al.*, 2007; Haas *et al.*, 2012; Holzworth *et al.*, 2014; Wu *et al.*, 2016; Zhang *et al.*, 2016; Zhang *et al.*, 2018). The models derived from SWAT were all based on semi-distributed hydrological models using hydrologic response units and did not perform better in estimating non-point source pollution (e.g., Pohlert *et al.*, 2007; Bosch *et al.*, 2011 ;Wu *et al.*, 2016). A coupler was used to couple two models for LandscapeDNDC-CMF (e.g., Haas *et al.*, 2012; Schroeck *et al.*, 2019). Compared with other models, the Catchment Nutrient Management Model - DeNitrification-DeComposition (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 showed good performance for simultaneously simulating various variables, including ecosystem productivity, hydrological nitrogen losses and nitrate discharge in streams, and emissions of gaseous carbon and nitrogenous gases (Zhang *et al.*, 2018). Therefore, the CNMM-DNDC has the capacity to evaluate the sustainability of ecosystems with simultaneous simulations of various variables closely related to both productivity and environmental hazards.

However, as a process-oriented hydro-biogeochemical model designed to be applicable to different climate zones, soils, land uses and field management practices, CNMM-DNDC testing is still lacking due to limited observations for model validation. In this study, the model was applied to a catchment in seasonally frozen regions located on the eastern Tibetan Plateau (TP) with the land use types of alpine wetlands, meadows and forests to test its ability to simulate hydro-biogeochemical 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 land surface of the Northern Hemisphere (Jiang *et al.*, 2020). In addition, the soil freeze-thaw cycles that occur in these mid-high latitude regions exert important influences on soil thermal dynamics, as well as on related hydrological processes, thus increasing the availability of substrates and stimulating the processes of CH_4 and N_2O production and emissions in soils (e.g., 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, hydrological processes and CH_4 and N_2O fluxes in seasonally frozen regions. Filling this gap is especially necessary to broaden model applicability.

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To test the above hypothesis, the catchment simulation in the Rierlangshan was conducted using a unique experimental dataset, which was obtained by Zhang *et al.* (2018a, 2019) and Yao *et al.* (2019) for the catchment that involved three typical alpine ecosystems, wetlands, meadows and forests, on the eastern TP. 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 frozen regions; (ii) compare the performances of the original and modified models in simulating the soil profile temperature, topsoil moisture and CH_4 and N_2O fluxes in three typical alpine ecosystems in the Rierlangshan catchment with field observations, and (iii) evaluate the model performance in simulating the effects of wetland degradation on CH_4 and N_2O fluxes. Therefore, the validated model with modifications provides a mechanism for not only interpreting observations but also predicting the CH_4 and N_2O fluxes in alpine ecosystems.

2 Materials and methods

2.1 Model description

2.1.1 Overview of the CNMM-DNDC model

The CNMM-DNDC is a process-oriented model developed for simulating hydro-biogeochemical interactions at the catchment or site scale, and this model is designed following the basic theories of physics, chemistry, and biogeochemistry and has the capacity to simulate the complex transport and transformation of water, nitrogen and carbon in terrestrial 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 discharge in streams from an entire catchment or individual landscape unit (Zhang *et al.*, 2018b).

The model was established to address the bottleneck issue associated with most biogeochemical models, i.e., the inability to simulate the lateral flows of water and nutrients, by incorporating the core biogeochemical processes of DNDC (including the processes of decomposition, nitrification, denitrification and fermentation) into the hydrological framework of the CNMM. In the CNMM-DNDC, the processes related to the production of N_2O include nitrification and denitrification, which occur simultaneously at aerobic and anaerobic microsites, 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 determined by the soil redox potential (Eh) using the Nernst equation (Li, 2007). The “hole in the pipe” concept was applied to calculate N_2O production during nitrification, which is influenced by the soil moisture, temperature and pH. The production of N_2O during denitrification was predicted with Michaelis-Menten kinetics and Pirt functions following the reaction chain of denitrification. The predicted CH_4 flux was influenced by CH_4 production, oxidation and transportation. Methane production and oxidation occurred simultaneously and were determined by the sizes of yhr aerobic (production) and anaerobic (oxidation) microsites, which were defined by an Eh calculator in terms of an “anaerobic balloon” (“CH_4 balloon”). The predicted CH_4 production was calculated from the carbon

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substrates resulting from decomposed soil organic carbon (SOC) and plant root biomass with the effects of soil temperature. Three pathways of CH_4 transportation in soils were included in the model: plant-mediated transport, ebullition and diffusion. For more details, please see Li. (2007) and Zhang *et al.* (2018b).

2.1.2 Modifications of the CNMM-DNDC model

In this study, to replace the original thermal module that involved simple parameterizations with a physically based model describing the soil thermal regime in the presence of freeze-thaw cycles, the Northern Ecosystem Soil Temperature model was incorporated into the CNMM-DNDC at the code level (Zhang *et al.*, 2003). The modified model explicitly described the energy exchange within the soil-vegetation-atmosphere system and the active layer dynamics (Zhang *et al.*, 2003; Deng *et al.*, 2014). These modifications are indispensable for accurately simulating freeze-thaw cycles in seasonally frozen regions, which are crucial for characterizing the active layer and soil thermal dynamics, soil hydrology and nitrogen or carbon cycling in these regions.

The thermal dynamics of the soil and snow were calculated by the one-dimensional heat conduction equation (Eq. 1), which was solved numerically using Eqs. 2–4. In the above equations, C (J m^{-3} ℃$^{-1}$), k (W m^{-1} ℃$^{-1}$), T (℃) and G (W m^{-2}) denote 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), Δt is the time step of the calculation, and l denotes the soil layer l. S is the internal heat exchange due to freezing or thawing (W m^{-3}) when the soil temperature is around 0 ℃. The soil temperature changes affected by freezing or thawing were determined on the basis of energy conservation, which indicated that the latent heat released during freezing equalled the amount of heat required for the increased soil temperature and vice versa. The soil heat capacity (C, J m^{-3} ℃$^{-1}$) is the weighted average of five constituents in the volumetric fraction (θ), including organic matter (2.5×10^6), minerals (2.0×10^6), water (4.2×10^6), ice (2.1×10^6) and air (1.2×10^3) (Eq. 5). The thermal conductivity (k, W m^{-1} ℃$^{-1}$) is the geometric mean of the thermal conductivities of the above five constituents (Eq. 6), with values of 0.25, 2.9, 0.57, 2.2 and 0.025 W m^{-1} ℃$^{-1}$ for organic matter, minerals, water, ice and air, respectively. The upper and lower boundary conditions of the thermal dynamics were determined by the surface energy balance and the defined geothermal heat flux at a soil depth of 35 m.

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

$$C_l\frac{\Delta T_l}{\Delta t} = \frac{G_{l-1,\,l} - G_{l,\,l+1}}{D_l} + S_l \quad (2)$$

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

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

$$C_l = \sum_{j=1}^{5} C_{l,\,j}\theta_{l,\,j} \quad (5)$$

$$k_l = \prod_{j=1}^{5} k_{l,\,j}^{\theta_{l,\,j}} \quad (6)$$

Descriptions of the processes related to soil thermal dynamics are detailed in Zhang *et al.* (2018b). The modified CNMM-DNDC was able to simulate the thermal dynamics in seasonally frozen regions as well as their impacts on biogeochemical processes, especially the emissions of nitrogen and carbon gases.

2.2 Catchment and field descriptions

The study area is the Rierlangshan catchment (34°02′N, 102°43′E) on the eastern TP with an area of 189 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 upper Yangtze River (Zhang *et al.*, 2018a). This region is subject to a cold humid continental monsoon climate, and it had an annual mean air temperature of 1.6 ± 0.7 °C and average annual precipitation of 649 ± 94 mm in 1980–2012 as observed at the Zoige Meteorological Station (~80 km south of the catchment) (Ma *et al.*, 2018). The catchment consists of alpine wetlands, meadows and forests (Yao *et al.*, 2019). The alpine wetlands in the catchment are part of the Zoige wetland and are degraded due to anthropogenic drainage and climate warming (Dong *et al.*, 2010; Li *et al.*, 2014). Degraded alpine wetlands are commonly distributed throughout the Zoige wetland, and nearly 83% of the permanently inundated wetlands have been converted into “wet grassland” (Xiang *et al.*, 2009; Li *et al.*, 2014).

CH_4 and N_2O fluxes were manually measured weekly or twice per week using the gas chromatograph-based static opaque chamber method at three sites in alpine wetlands (34°02′6.53″N, 102°43′29.66″E, 3304 m a.s.l.), 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 Rierlangshan catchment from 2013 to 2015 (Zhang *et al.*, 2018a; Yao *et al.*, 2019; Zhang *et al.*, 2019) (Fig. S1). The alpine meadow site is located on a north-facing slope with a slope gradient of 11° and neighbours the alpine wetland site at the slope base with a gentle slope of 2°. In addition, 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 field observations of the CH_4 and N_2O fluxes and the relevant auxiliary variables are described in Zhang *et al.* (2018a), Yao *et al.* (2019), Zhang *et al.* (2019) and Table S1 (online supplementary materials).

2.3 Model simulation

The modified CNMM-DNDC was applied in the Rierlangshan catchment with the three alpine ecosystems: wetlands, meadows and forests. The dataset required for the catchment simulation included (1) a digital elevation model (DEM) with a resolution of 30 × 30 m^2 from the geospatial data cloud (Fig. S1; http://www.gscloud.cn/); (2) a map of alpine ecosystems, including wetlands, meadows and forests; (3) a climate dataset of hourly weather data (air temperature, precipitation, wind speed, solar radiation, longwave radiation, and humidity), which were obtained from the meteorological station in the target 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: 10th June, 2020) for other years; (4) a soil properties dataset of the observed clay fraction, organic matter content, total nitrogen, 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;

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Zhang *et al.*, 2019); and (5) a management practices dataset including grazing time and intensity for the alpine wetlands and meadows. In addition, other required soil inputs of field capacity, wilting point and saturated hydrological conductivity were calculated by pedo-transfer functions (Li *et al.*, 2019). The simulated soil profile (0−35 m depth) was divided into 23 layers. The thicknesses of the top 20 layers were 1, 5 and 10 cm for the top 10 layers, middle 2 layers, and other 8 layers, respectively. The thicknesses of the last three layers were 0.5, 3.5 and 31 m. The geothermal heat flux in the catchment was estimated at 0.053 W m^{-2} (Pollack and Chapman, 1977). Therefore, using the database, a catchment simulation of hydro-biogeochemical processes was performed with spatial and temporal resolutions of 30×30 m^2 and 3 hours, respectively, by the modified CNMM-DNDC.

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 index (NSI), (iii) the determination coefficient (R^2) and slope of the zero-intercept univariate linear regression (ZIR) of the observations against the simulations, and (iv) the model relative bias (MRB) (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 ranging from 0 to 1. An NSI value (ranging from minus infinity to 1) closer to 1 was better. Better model performance was indicated by a slope and an R^2 value that were both closer to 1 in a significant ZIR. For more details on these criteria, refer to the online supplementary materials (Eqs. S1−4 in Table S2). In addition, the SPSS Statistics Client 19.0 (SPSS Inc., Chicago, USA) and Origin 8.0 (OriginLab, Northampton, MA, USA) software packages were applied for the statistical analysis and graphical comparison.

3 Results

3.1 Model validation

3.1.1 Soil temperature and moisture

The simulated soil profile temperatures of the three typical 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 from the field observations for various soil depths, with IA, NSI, and ZIR slopes and R^2 values of 0.91−1.00, 0.68−0.99, 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 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. S3).

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For the topsoil moisture, the simulated soil moisture dynamics were comparable to those from the field observations, with IA and NSI values of 0.59−0.83 and -0.94−0.32 for the three alpine ecosystems, respectively (Fig. 2 and Table 1). In comparison to the other alpine ecosystems, the alpine wetlands had higher soil moisture, which ranged from 0.41 to 0.98 and from 0.38 to 0.93 for the observations and simulations in the water-filled pore space (WFPS), respectively. The soil moisture values of the alpine meadows and forests were highly variable and depended on the variation trend in precipitation for both observations and simulations. However, an underestimation of soil moisture in the winter period occurred for both alpine meadows and forests due to a possible overestimation of evapotranspiration. The performances of the modified model in simulating the soil profile temperature and topsoil moisture indicate that the modified CNMM-DNDC can reliably predict the soil thermal dynamics and water movement in the three alpine ecosystems at the catchment scale, which is crucial for correctly simulating soil hydrology, plant growth and biogeochemical processes.

3.1.2 Methane fluxes

The daily observed CH_4 emissions from the alpine wetlands were highly variable and showed a clear seasonal cycle, with intensive CH_4 emissions from May to November and weak emissions in other periods (Fig. 3a). The observed alpine 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. 4a and 5a). The original model significantly overestimated CH_4 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, with an IA of 0.57−0.88 for the three alpine ecosystems (Figs. 3−5 and Table 1). However, the CH_4 uptake rates during the dormant season were obviously underestimated by the modified model at both sites, especially at the alpine forest site, which 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^{-1} yr^{-1} and the modelled values ranged from -1.90 to 31.0 kg C ha^{-1} yr^{-1} (Fig. 6a). These results indicate that the modified CNMM-DNDC successfully simulated the CH_4 fluxes of the three typical alpine ecosystems at the catchment scale and showed the capacity to predict the effects of wetland degradation on CH_4 emissions.

3.1.3 Nitrous oxide fluxes

The daily observed N_2O emissions from the alpine wetlands were higher than those from the alpine meadows but lower than those from the alpine forests (Figs. 3b, 4b and 5b). Similar seasonal patterns of N_2O fluxes were observed for the three alpine ecosystems with intensive emissions in the growing season. The N_2O emission peak during the dormant season was observed in the alpine meadows and, was the major contributor to annual emissions. The modified CNMM-DNDC generally captured the seasonal dynamics of daily N_2O fluxes with an IA of 0.26−0.47 for the three alpine ecosystems (Figs. 3−5 and Table 1), but the N_2O emissions from the alpine wetlands were significantly overestimated by the original model. For the modified model, the simulated N_2O emissions from the alpine wetlands and forests showed obvious seasonal patterns with higher emissions during the growing season, but no abrupt emission peak was captured at the end of the growing season 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 emissions were not well simulated. The observed cumulative N_2O emissions ranged from 0.14 to 0.58 kg N ha^{-1} yr^{-1} and the modelled values ranged from 0.12 to 0.32 kg N ha^{-1} yr^{-1} (Fig. 6b). These results indicate that the modified CNMM-DNDC showed the potential to estimate N_2O emissions in seasonally frozen regions and thus was able to assess the influences of wetland degradation on N_2O emissions.

3.2 Annual aggregate emissions of CH_4 and N_2O

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_2eq ha^{-1} yr^{-1} 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_2eq ha^{-1} yr^{-1} for the alpine wetlands, meadows and forests, respectively) (Fig. 6c). However, the original model significantly overestimated the aggregate emissions due to the high predicted CH_4 and N_2O emissions. In comparison, the degraded wetlands functioned as the sources of aggregate emissions of CH_4 and N_2O, but the aggregate emissions from adjacent wet alpine meadows were much lower. Zhang *et al.* (2019) found that annual CH_4 emissions from permanently inundated wetlands were 7.1 times higher than those from degraded wetlands with seasonal inundation. Assuming N_2O emissions were zero for permanently inundated wetlands (e.g., Kolb and Horn, 2012; Hatano, 2019), the aggregate emissions of CH_4 and N_2O were estimated at 10.8 Mg CO_2eq ha^{-1} yr^{-1} for natural alpine wetlands based on observations. For the virtual experiment of annually inundated wetlands, the simulated aggregate emissions of CH_4 and N_2O were 7.2 Mg CO_2eq ha^{-1} yr^{-1} with CH_4 and N_2O emissions of 158 kg C ha^{-1} yr^{-1} and 0.0 kg N ha^{-1} yr^{-1}, respectively (Fig. 6). These consistent results also illustrate that the modified model performed well in capturing the characteristics of the CH_4 and N_2O emissions from the three typical alpine ecosystems in seasonally frozen regions. In addition, wetland degradation resulted in decreased CH_4 emissions but increased N_2O emissions. However, the increased N_2O emissions could be totally offset by the reduced CH_4 emissions, thus finally leading to the decreased aggregate emissions of CH_4 and N_2O from degraded wetlands than permanently inundated wetlands but still much higher than those of adjacent wet alpine meadows.

4 Discussions

4.1 Model performance in simulating thermal dynamics

The soil freeze-thaw cycles in seasonally frozen regions determine the soil profile temperature and hydrological processes, which are key factors that regulate the cycling of nitrogen and carbon (e.g., Zhang *et al.*, 2015; Hugelius *et al.*, 2020). Therefore, improving the scientific processes of soil thermal dynamics in the presence of active layer dynamics is

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essential for applying the CNMM-DNDC to simulate the biogeochemical processes in seasonally frozen regions, which are sensitive and vulnerable to climate change and human activities (Hatano, 2019; Hugelius *et al.*, 2020; Jiang *et al.*, 2020). The original model adopted a relatively simple module with an empirical function to calculate thermal transportation within the soil-vegetation-atmosphere system and did not consider the effects of freeze-thaw cycles on soil temperature and moisture. The newly incorporated module was based on explicit energy conservation and exchange in the soil profile and successfully captured the variations in soil temperature and topsoil moisture for the three alpine ecosystems during the freeze-thaw period. Compared with other models applied in seasonally frozen regions at different scales, the modified CNMM-DNDC simulated soil profile temperature influenced by soil hydrological processes equally well (e.g., Zhang *et al.*, 2002; Deng *et al.*, 2014; Guo *et al.*, 2015; Jiang *et al.*, 2020). In addition, the simulated lower soil frozen depth for the observed alpine wetland was primarily attributed to the higher soil profile moisture level, as the thermal conductivity and heat capacity for water-filled pores were higher than those for air-filled pores. These results indicate the efficiency of the incorporated module in simulating soil thermal dynamics and related hydrological processes in seasonally frozen regions.

4.2 Model performance in simulating CH_4 fluxes

Compared with the annually inundated wetlands, the seasonally inundated wetlands had relatively low observed and simulated CH_4 emissions due to the significant influences of the water table level on CH_4 emissions (e.g., Hatano, 2019; Zhang *et al.*, 2019). The CH_4 emissions simulated by the CNMM-DNDC were determined by the processes of production, oxidation and transpiration under the concept of a CH_4 balloon. The unsaturated soil with moisture levels ranging from 0.41 to 0.98 WFPS resulted in a small CH_4 balloon and thus reduced CH_4 production. At the same time, relatively dry conditions caused the upper soil layer to act as an efficient oxidative methanotrophic barrier for the diffusion of CH_4 from the subsoil and thus decreased CH_4 emissions (Kandel *et al.*, 2018; Tan *et al.*, 2020). In addition, the highly fluctuating CH_4 emissions simulated by the modified model were also attributed to the high dependency of CH_4 production on soil moisture, which controlled the size of the CH_4 balloon. Theoretically, the CH_4 emissions simulated by the original model should not have been higher than those simulated by the modified model due to the lower predicted soil moisture level. The overestimated CH_4 emissions simulated by the original model were mainly attributed to the overestimated soil temperature due to their influences on mineralized substrates for CH_4 production, as well as the processes of CH_4 production. This result implies that global warming may trigger intensive CH_4 emissions from degraded wetlands, which could partly serve as a trade-off for the decreased CH_4 emissions due to the lower water table level in degraded wetlands. Both observations and simulations showed that the CH_4 uptake in alpine forests was higher than that in alpine meadows, which was mainly attributed to the high SOC content and low soil clay fraction of the alpine forests in the simulation. Methane uptake by upland soils is a biological process governed by the availability of CH_4 and oxygen as well as the activity and quantity of methanotrophic bacteria in soils (e.g., Liu *et al.*, 2007; Zhang *et al.*, 2014). In the model, the simulated CH_4 uptake was positively related to the SOC content, which is closely related to the population size of methanotrophic bacteria. On the other hand, soil permeability affects gas diffusion into the soil and thus CH_4 uptake (e.g., Liu *et al.*, 2007). For the CNMM-DNDC, the clay fraction, which is regarded as a key factor regulating soil permeability, showed a negative relationship with CH_4 uptake in the model. Thus, the SOC content, as well as the soil clay fraction, contributed to the differences in CH_4 uptake from alpine meadows and forests. As the simulated dynamic characteristics of CH_4 uptake were primarily regulated by soil temperature and moisture, the effects of low soil temperature (< 0.0 ℃) on CH_4 uptake rates resulted in obvious underestimations in the dormant season for both alpine meadows and forests. Therefore, an improved parameterization for simulating CH_4 uptake under low soil temperatures is required for the model to better capture the dynamics of CH_4 uptake in the dormant season.

4.3 Model performance in simulating N_2O 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 are large carbon reserves and play a crucial role in mitigating global warming (e.g., Deng *et al.*, 2014; Kang *et al.*, 2020; Tan *et al.*, 2020). The intentional drainage of annually inundated wetlands alters not only the water regime but also nutrient availability (e.g., Hoffmann *et al.*, 2016). The simulated relatively low soil moisture for the alpine wetlands stimulated the decomposition of SOC and nitrogen (or peat oxidation) under aerobic conditions, thus improving nitrogen mineralization for nitrification and denitrification and enhancing N_2O emissions (e.g., Tan *et al.*, 2020; Zhang *et al.*, 2020). The intensive N_2O emissions simulated by the original model resulted from the overestimated soil temperature for the alpine wetlands, as well as the lower predicted soil moisture, which not only facilitated soil mineralization but also provided favorable oxygen conditions for N_2O production. This result also indicates that global warming may significantly increase N_2O emissions from seasonally inundated wetlands. Field studies showed that high SOC concentrations could stimulate the processes of mineralization and nitrification 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 forests was more than twice that in the observed alpine meadows. Thus, the high SOC content at the alpine forest site provided more available nitrogen through mineralization and thus stimulated the nitrification processes in the simulation. Furthermore, the seasonal grazing that occurred in the alpine meadows resulted in constant loss of available nitrogen and thus hindered the N_2O emissions from the biological processes in the simulation. The soil freeze-thaw cycles that occurred in seasonally frozen regions, which were included in the modified CNMM-DNDC, not only increased the availability of nitrogen and carbon substrates by disrupting of soil aggregates but also affected the structure, population and activity of the microbes, and thus influencing the emissions of N_2O (e.g., Song *et al.*, 2019). The model set threshold values of soil temperature to trigger the decomposition of microbes during the freezing period and stimulate the production of NO, N_2O and N_2 using substrates derived from microbial decomposition during the thawing period. However, the dynamics of peak emissions due to freeze-thaw cycles were inconsistent with those from the field observations. Thus, improvements are required to optimize the parameterization scheme to better capture the dynamic characteristics. In addition, the peak emissions during the freeze-thaw period were not captured by the original model due to the significantly overestimated soil temperature. The low evaluation statistics for the daily fluxes, especially for the alpine forests, were also attributed to the underestimation of background emissions, which resulted from both measurement errors due to low fluxes around detection limits and model deficiencies in the simulation of tight nitrogen cycling in natural ecosystems. The 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, hydrology, nitrogen and carbon cycling and related greenhouse gas emissions in seasonally frozen regions.

4.4 Implications for degraded alpine ecosystems

The typical natural wetland alpine ecosystems, which are annually inundated, act as greenhouse gas sinks or are neutral (e.g., Cai., 2012; Tan *et al.*, 2020). A previous study showed that more than 90% of the annually inundated wetlands on the TP have been degraded and become seasonally inundated or wet alpine meadows due to intentional drainage for grazing since the 1960s (Wei *et al.*, 2015). Both the observations and simulations showed that in comparison to annually inundated wetlands, wetland degradation induced by drainage stimulated N_2O emissions to a small extent but reduced CH_4 emissions to a large extent. Thus, compared to that from natural wetlands, the aggregate emissions of CH_4 and N_2O from degraded wetlands were largely reduced but still higher than those of adjacent wet alpine meadows. These results were consistent with the field observations of CH_4 and N_2O emissions along different water table transects in the Zoige peatland, which were primarily driven by soil water content and SOC (Zhang *et al.*, 2020). The decline in the water table induced by intentional drainage resulted in recessive succession of the vegetation for the Zoige wetland with a typical mode of marsh, marsh meadow and meadow (Xiang *et al.*, 2009). Thus, one may deduce that the degradation of annually inundated wetlands at a large-scale might have greatly reduced the aggregate emissions of CH_4 and N_2O from the Zoige wetland, especially for CH_4. However, a recent meta-analysis showed that the reduction in the aggregate emissions of CH_4 and N_2O due to draining may be completely offset by the decreased net CO_2 uptake (Tan *et al.*, 2020). For natural wetlands, anaerobic conditions under high a water table inhibit litter decomposition, and thus, a large amount of organic matter is sequestered (Nahlik and Fennessy, 2016). When the annually inundated wetlands degrade to seasonally inundated wetlands or meadows, the rate of peat soil oxidation is enhanced, thus significantly increasing ecosystem respiration and resulting in a shift from net sinks of greenhouse gas emissions to notable sources (Tan *et al.*, 2020). Consistent with the results of the meta-analysis, the simulation showed that the loss rate of SOC (consisting of microbes, humads and humus) was much higher for degraded wetlands than for other typical alpine ecosystems. These results also indicate the large risk of soil carbon loss due to intentional drainage, which has been sequestered for a long time. The simulation by the modified CNMM-DNDC showed that the model has the capacity to simulate hydro-biogeochemical processes in seasonally frozen regions for various alpine ecosystems.

5 Conclusions

To apply the process-oriented hydro-biogeochemical model Catchment Nutrient Management Model - DeNitrification-DeComposition (CNMM-DNDC) in seasonally frozen regions, an improved module of soil thermal dynamics for describing

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the soil thermal regime in the presence of freeze-thaw cycles was incorporated in this study. Using the unique experimental dataset obtained for the Rierlangshan catchment with the typical alpine wetland, meadow and forest ecosystems, the modified model was evaluated for simulating soil thermal dynamics (soil profile temperature), topsoil moisture and methane (CH_4) and nitrous oxide (N_2O) fluxes for the three ecosystems and the effects of wetland degradation on CH_4 and N_2O fluxes in seasonally frozen regions of the Tibetan Plateau. The simulations showed acceptable performances for the above variables, indicating the capacity of the modified model to simulate the processes of thermal dynamics, hydrology, and nitrogen and carbon cycling in seasonally frozen regions. Both the observed and simulated CH_4 and N_2O fluxes from alpine wetlands and meadows, as well as the results from the simulated annually inundated wetlands, indicate that wetland degradation due to intentional drainage resulted in a significant reduction in the aggregate emissions of CH_4 and N_2O. Reduced soil moisture and lower soil organic carbon contents were the primary factors for the decreased aggregate emissions of CH_4 and N_2O. In addition, the simulated intensive losses of soil organic carbon for the alpine wetlands suggest the inhibitory effects of wetland degradation on soil carbon sequestration but stimulatory influences on net greenhouse gas emissions. This study implies that hydro-biogeochemical model, such as the modified CNMM-DNDC, are able to predict soil thermal dynamics and cycling of nitrogen and carbon in seasonally frozen regions with an improved physical-based soil thermal module.

Data availability

The model, input and output databases can be obtained from the first author and all the observed data sets used in this study can be available from the co-authors.

Author contribution

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

Competing interests

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.

Item	Ecosystem	*n*	IA		NSI		Slope		R^2[c]		P	
			O[a]	M[b]	O	M	O	M	O	M	O	M
Soil temperature												
5 cm	Meadow	500	0.90	0.96	0.82	0.95	0.84	1.09	0.89	0.96	< 0.001	< 0.001
	Forest	48	0.85	0.91	0.37	0.68	0.64	0.83	0.68	0.73	< 0.001	< 0.001
10 cm	Wetland	366	0.90	0.98	0.57	0.92	0.72	1.07	0.81	0.93	< 0.001	< 0.001
	Meadow	500	0.93	0.99	0.71	0.95	0.80	1.08	0.85	0.96	< 0.001	< 0.001
20 cm	Wetland	366	0.82	0.99	0.18	0.96	0.64	1.05	0.66	0.97	< 0.001	< 0.001
	Meadow	500	0.87	0.99	0.48	0.97	0.74	1.06	0.76	0.98	< 0.001	< 0.001
50 cm	Wetland	366	0.66	0.99	-1.01	0.97	0.51	1.05	0.43	0.97	< 0.001	< 0.001
	Meadow	401	0.70	1.00	-0.48	0.99	0.58	1.06	0.53	1.00	< 0.001	< 0.001
70 cm	Wetland	366	0.58	0.98	-2.23	0.93	0.47	1.05	0.38	0.93	< 0.001	< 0.001
	Meadow	401	0.64	1.00	-1.19	0.99	0.54	1.03	0.49	1.00	< 0.001	< 0.001
90 cm	Wetland	366	0.52	0.98	-4.07	0.90	0.44	1.03	0.36	0.90	< 0.001	< 0.001
Soil moisture	Wetland	74	0.63	0.83	-1.65	0.20	1.31	1.13	–	0.60	–	< 0.001
	Meadow	128	0.78	0.78	0.28	0.32	0.96	0.93	0.30	0.41	< 0.001	< 0.001
	Forest	40	0.48	0.49	-1.04	-0.80	1.21	1.19	–	–	–	–
Daily CH_4 flux	Wetland	180	0.37	0.74	-11.1	-0.73	0.46	0.87	–	–	–	–
	Meadow	168	0.87	0.88	0.42	0.38	1.09	0.94	0.44	0.39	< 0.001	< 0.001
	Forest	49	0.59	0.57	-2.79	-3.39	0.92	0.79	–	–	–	–
DailyN_2O flux	Wetland	180	0.01	0.26	-323	-0.07	0.01	0.59	–	–	–	–
	Meadow	168	0.23	0.44	-0.16	-1.76	0.99	0.35	–	–	–	–
	Forest	58	0.47	0.47	-1.85	-1.64	0.44	0.47	–	–	–	–

[a] O indicates the simulations by the original model. [b] M indicates the simulations by the modified model. [c] "–" indicated no value.

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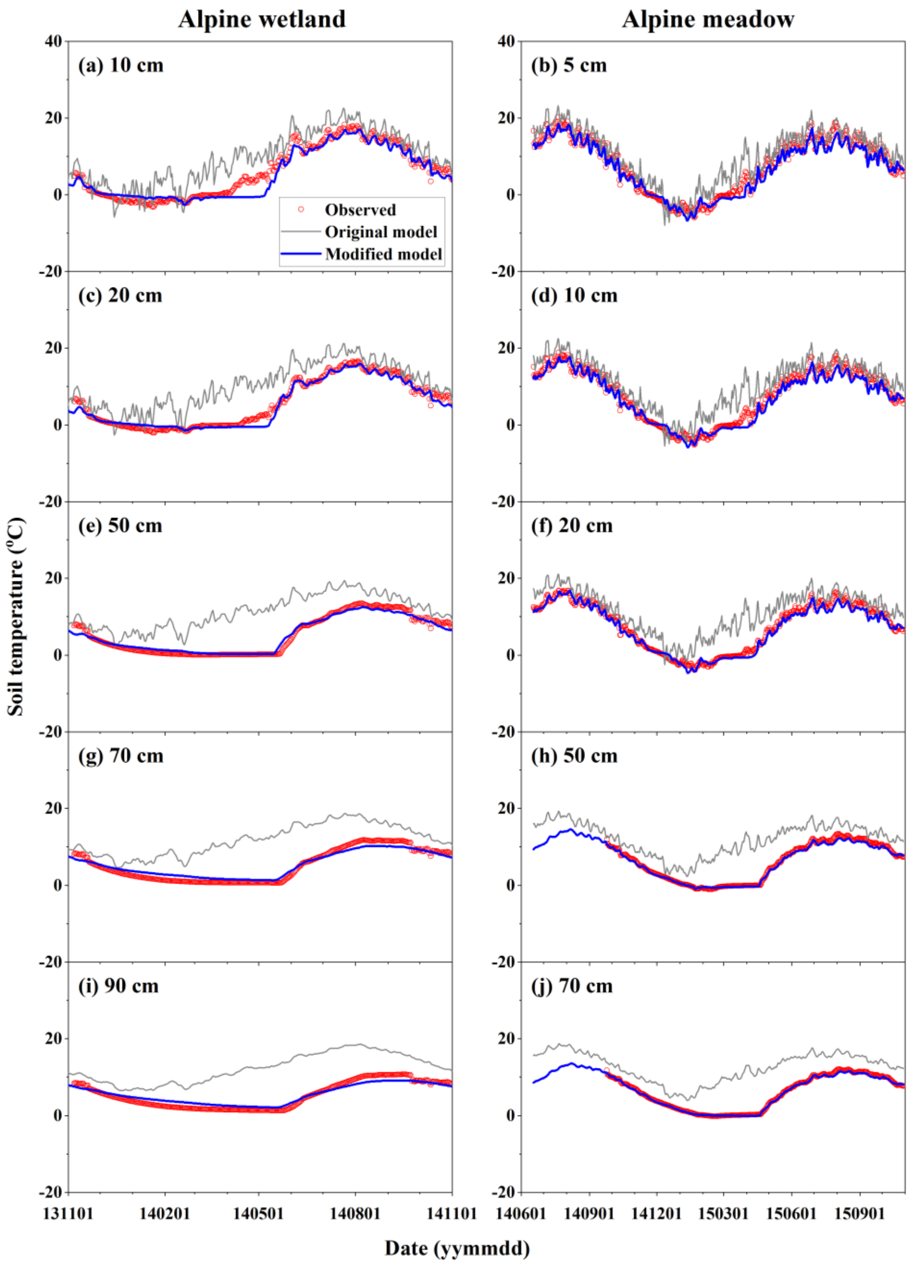

Figure: 1 Observed and simulated daily profile soil temperature from the alpine wetlands and meadows by the original and modified models. The legends in panel a apply for all panels.

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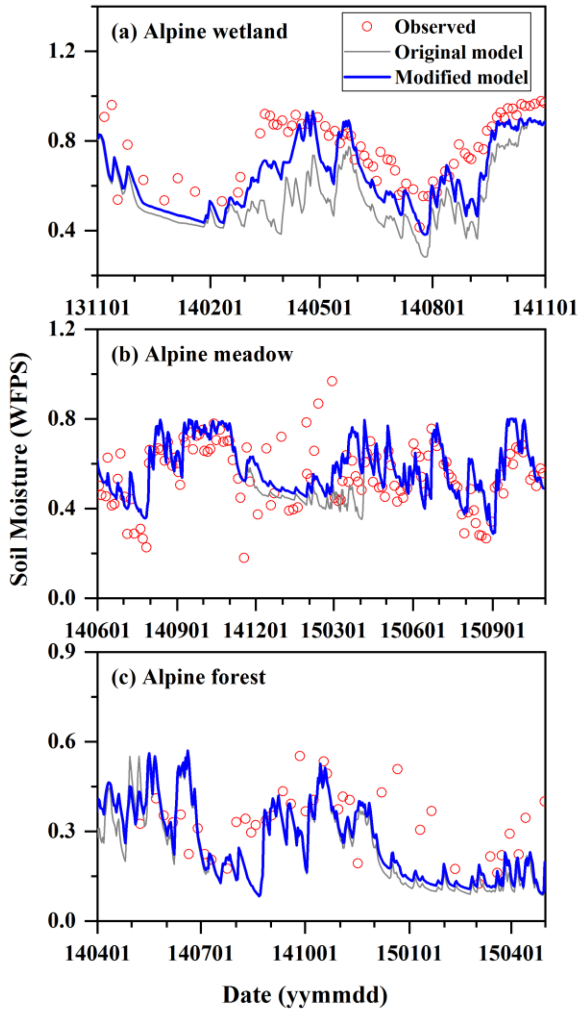

Figure: 2 Observed and simulated daily topsoil (0–6 cm) moisture in the water-filled pore space (WFPS) from the alpine wetlands, meadows and forests by the original and modified models. The legends in panel a apply for all panels.

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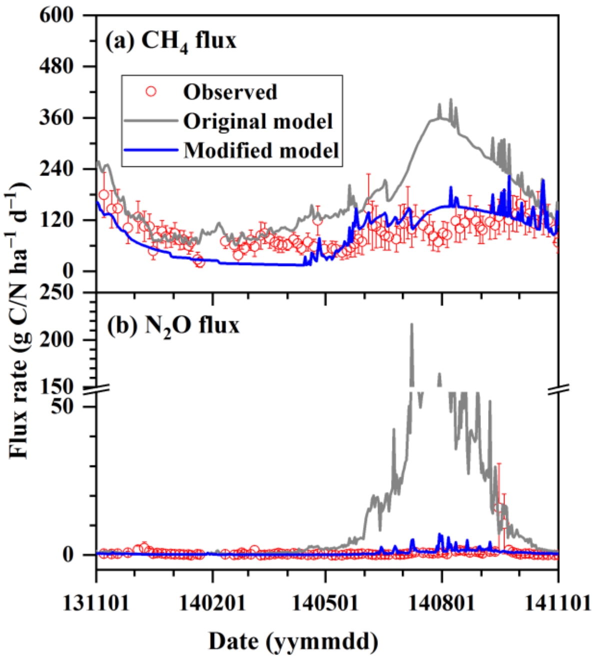

Figure: 3 Observed and simulated daily methane (CH_4) and nitrous oxide (N_2O) fluxes from the alpine wetlands by the original and modified models. The vertical bar for each observation indicates the standard error of six spatial replicates. The legends in panel a apply for all panels.

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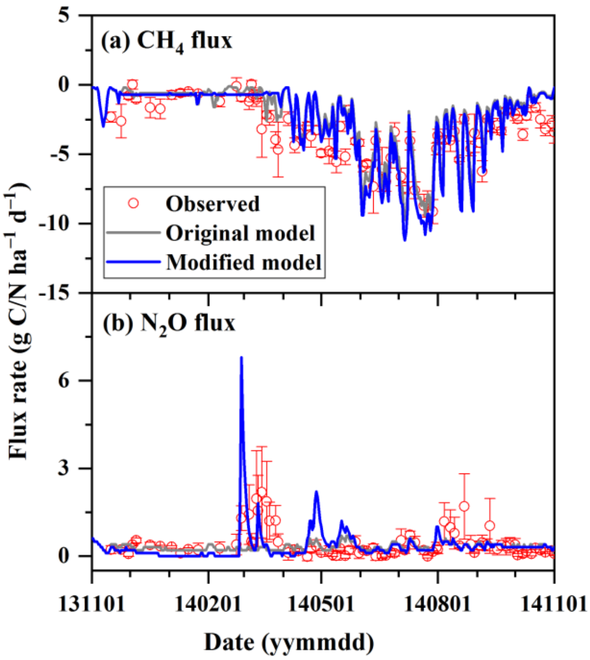

591
592 **Figure: 4 Observed and simulated daily methane (CH_4) and nitrous oxide (N_2O) fluxes from the alpine meadows by the original**
593 **and modified models. The vertical bar for each observation indicates the standard error of four spatial replicates. The legends in**
594 **panel a apply for all panels.**

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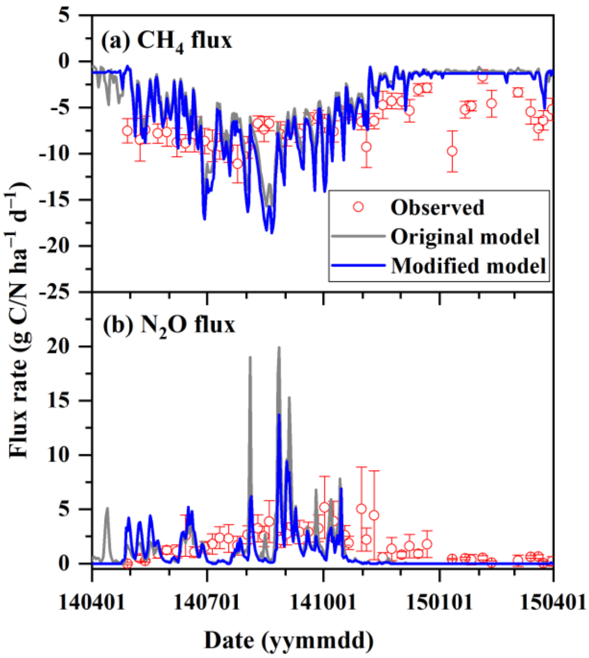

Figure: 5 Observed and simulated daily methane (CH_4) and nitrous oxide (N_2O) fluxes from the alpine forests by the original and modified models. The vertical bar for each observation indicates the standard error of four spatial replicates. The legends in panel a apply for all panels.

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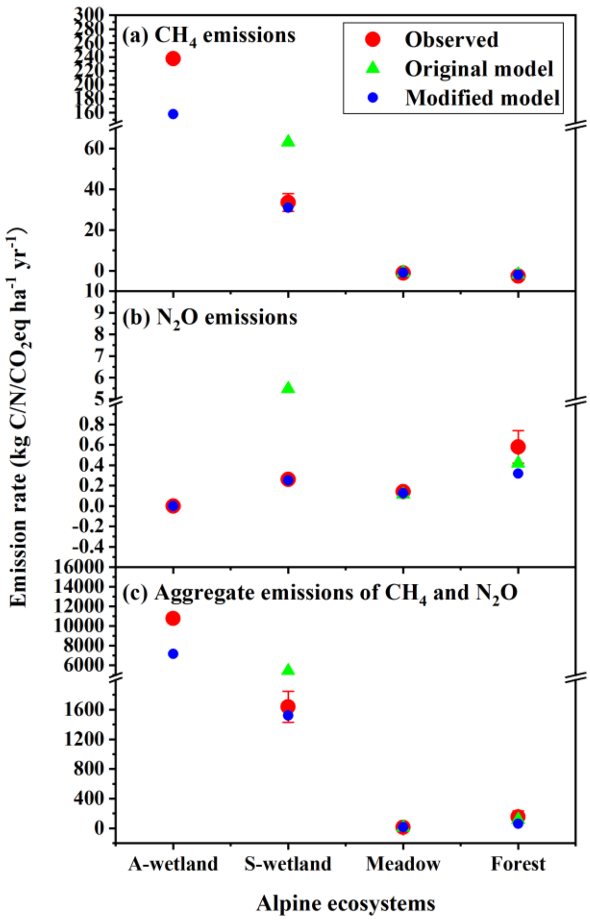

Figure: 6 Observed and simulated annual emissions of methane (CH_4), nitrous oxide (N_2O) and aggregate emissions of both from the annually inundated wetlands (A-wetland), seasonally inundated wetlands (S-wetland), alpine meadows and forests. The legends in panel a apply for all panels.