Factors that influence nitrous oxide emissions from agricultural soils as well as their representation in simulation models: A review

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Table S1. Factors that influence N_2O emissions from peer-reviewed literature.

Review literature	Micro	SOC	N	WFPS	Texture	T	pH & salinity	Tillage	Crops	Fertilizer	Irrigation	Harvest & residues	Length	Types
Abdalla et al. [1]			√	√		√		√	√	√		√		
Aguilera et al. [2]		√	√	√	√	√	√	√	√	√	√		√	
Beauchamp [3]	√	√	√	√	√	√	√	√	√	√	√	√		
Bremner [4]	√	√	√	√		√	√							
Bouwman et al. [5]		√	√	√	√	√	√		√	√			√	
Butterbach_Bahl et al. [6]	√	√	√	√	√	√	√		√					
Cameron et al. [7]		√	√	√	√	√	√			√				
Charles et al. [8]		√	√	√	√	√	√	√	√					
Dalal et al. [9]		√	√	√		√	√			√				√
De Klein et al. [10]	√	√	√	√	√	√	√			√				
Eichner [11]	√	√	√	√	√	√	√	√	√	√	√	√		
Groffman [12]														√
Lesschen et al. [13]		√	√	√	√	√	√		√	√		√		
Meurer et al. [14]					√				√					
Mosier [15]		√	√	√	√	√	√		√	√	√			
Oertel et al. [16]		√	√	√	√	√	√		√					√
Saggar et al. [17]		√	√	√	√	√	√		√			√		√
Sanz_Cobena et al. [18]								√	√	√	√	√		
Signor et al. [19]		√	√	√	√	√		√		√		√		
Smith et al. [20]			√	√						√		√	√	
Smith [21]			√	√	√	√				√				
Snyder et al. [22]		√	√	√	√	√	√	√	√	√	√	√		
Stehfest & Bouwman [23]		√	√	√	√		√		√	√			√	
Stein & Yung [24]	√			√		√								
Trost et al. [25]	√	√		√	√			√		√	√			
Uchida et al. [26]	√			√	√			√		√				
Wang et al. [27]		√	√		√	√	√		√	√				
Xu et al. [28]		√	√	√	√				√	√		√		

*Micro: microbes; T: temperature; Length: length of measurement period; Types: types of measurements.

Model part:

1 The DAYCENT model

Nitrification process

DAYCENT calculates nitrification as a function of soil moisture, soil pH, soil temperature and soil NH_4^+ level (Eq.S1) [29, 30]. The equation (Eq.S1) calculates the total gas flux from nitrification (N_2O and NO_x), and N_2O emissions from nitrification is partitioned from NO_x by Eq.S17.

$$N^{N_2O} = F_\theta * F_{pH} * F_{Tmp} * (K_{mx} + N_{mx} * F_{NH_4}) \quad \text{(Eq. S1)}$$

F_θ, F_{pH}, F_{Tmp} , and F_{NH_4} are the effects soil moisture, soil pH, soil temperature and soil NH_4 level respectively on nitrification. K_{mx} is the N turnover coefficient, which is a function of the soil texture, soil N fertility, N fertilizer additions, and soil management practices. K_{mx} should be estimated with observed N_2O data or observed potential soil N mineralized data. N_{mx} is the maximum N_2O gas fluxes caused by nitrification with excess soil NH_4^+. Equations that calculate the effects of soil moisture, soil pH, soil temperature and soil NH_4 on nitrification are as follows:

$$F_\theta = \left(\frac{WFPS-b}{a-b}\right)^{d*\left(\frac{b-a}{a-c}\right)} * \left(\frac{WFPS-c}{a-c}\right)^{d} \quad \text{(Eq. S2)}$$

$$WFPS = \frac{(SW_{ly} * \rho_b)}{soil\ porosity} \quad \text{(Eq.S3)}$$

$$soil\ porosity = 1 - \rho_b / 2.65 \quad \text{(Eq.S4)}$$

$$F_{pH} = 0.56 + \frac{arctan(\pi * 0.45 * (-5 + pH))}{\pi} \quad \text{(Eq. S5)}$$

$$F_{Tmp} = -0.06 + 0.13 * e^{0.07 * soilt} \quad \text{(Eq. S6)}$$

$$F_{NH_4} = 1 - e^{-0.0105 * NH_4} \quad \text{(Eq. S7)}$$

Where SW_{ly} is gravimetric water content. ρ_b is soil bulk density. Parameters a, b, c, and d are empirical soil texture parameters according to the following Table S2:

Table S2. Soil texture parameters for nitrification rate.

Soil Texture	a	b	c	d
Sandy	0.55	1.70	-0.0070	3.22
Medium	0.60	1.27	0.0012	2.84

Denitrification process

The DAYCENT model calculates denitrification as a function of soil NO_3^- level, soil C, and soil moisture (Eq.S8) [29]. The equation S8 calculates the total gas flux (N_2O+N_2+NO_x) from denitrification, and N_2O emissions is differentiated from N_2 by Eq.S12 and from NO_x by Eq.S17.

$$D_t = min\left(F_d(NO_3), F_d(C)\right) * F_d(\theta) \quad \text{(Eq. S8)}$$

$F_d(NO_3)$ is the maximum total N gas flux for a given soil NO_3^- level, $F_d(C)$ is the maximum total N gas flux for a given soil respiration rate, and $F_d(\theta)$ is the effect of soil moisture on the denitrification rate. Equations for the calculation of the impacts of soil NO_3^- levels, soil C and soil moisture on denitrification are as follows:

$$F_d(NO_3) = 11000 + \frac{40000*atan(\pi*0.002*(NO_3-180))}{\pi} \quad \text{(Eq. S9)}$$

$$F_d(C) = \frac{24000}{\left(1+\frac{200}{e^{0.35*CO_2}}\right)} - 100 \quad \text{(Eq. S10)}$$

$$F_d(\theta) = \frac{a}{b^{\left(\frac{c}{b^{d*WFPS}}\right)}} \quad \text{(Eq. S11)}$$

Where a, b, c, and d are empirical soil texture parameters according to the following Table S3.

Table S3. Soil texture parameters for denitrification rate.

Soil Texture	a	b	c	d
Sandy	1.56	12	16	2.01
Medium	4.82	14	16	1.39
Fine	60.00	18	22	1.06

Partitioning N_2 from N_2O

After the total N_2 and N_2O emissions from denitrification is calculated by the equation (Eq.S8), the equation (Eq.S12) is used for partitioning N_2 from N_2O [29]:

$$R_{N_2/N_2O} = min\left(F_r(NO_3), F_r(C)\right) * F_r(\theta) \quad \text{(Eq. S12)}$$

$F_r(NO_3)$, $F_r(C)$, and $F_r(\theta)$ are the effect of soil NO_3^-, soil C and soil moisture on the ratio N_2/N_2O. Equations for calculation the effects of soil NO_3^-, soil C and soil moisture on N_2/N_2O ratio are as following:

$$F_r(NO_3) = (1 - \left(0.5 + \frac{1*\text{atan}\left(\pi*0.01*(NO_3-190)\right)}{\pi}\right)) * 25 \quad \text{(Eq. S13)}$$

$$F_r(C) = 13 + \frac{30.78*atan(\pi*0.07*(C-13))}{\pi} \quad \text{(Eq. S14)}$$

$$F_r(\theta) = \frac{1.4}{13^{\left(\frac{17}{13^{(2.2*WFPS)}}\right)}} \quad \text{(Eq. S15)}$$

Therefore, N_2 production during denitrification is:

$$D_{N_2} = \frac{D_t*R_{N_2/N_2O}}{1+R_{N_2/N_2O}} \quad \text{(Eq. S16)}$$

Partitioning NO_x from N_2O

Both nitrification and denitrification processes produce NO_x. The equation (Eq.S17) is used to differentiate NO_x from N_2O [31]:

$$NO_x = RNO_x * N_2O_{den} + RNO_x * N_2O_{nit} * P \quad \text{(Eq. S17)}$$

$$RNO_x = 15.2 + (35.5 * atan(0.68\pi(10D/D_o - 1.86)))/\pi \quad \text{(Eq. S18)}$$

RNO_x is the ratio of NO_x to N_2O fluxes, D/D_o is the soil gas diffusivity, which is calculated as a function of WFPS and soil physical properties, N_2O_{den} is the simulated N_2O flux from denitrification, N_2O_{nit} is the simulated N_2O flux from nitrification, and P is a pulse multiplier.

In the DAYCENT model, N_2O production from nitrification and denitrification is given by:

$$N_2O = N^{N_2O} + D_t - D_{N_2} - NO_x \quad \text{(Eq. S19)}$$

2 The DNDC model

Nitrification process

As a microbe-mediated process, the rate of nitrification in the DNDC model is regulated by soil temperature, soil moisture, soil pH and nitrifier's activity, which relies on two substrates, DOC and NH_4^+. The growth and death rates of nitrifiers are set as functions of DOC and soil moisture. The reaction rate of nitrification is subject to nitrifier's activity as well as other environmental factors such as NH_4^+ availability and soil pH. The nitrification-derived N_2O emissions is a fraction of the nitrification rate [32].

Relative growth (R_G) and death rates (R_D) of nitrifers:

$$R_G = 0.0166 * ([DOC]/(1.0 + [DOC]) + F_\theta/(1.0 + F_\theta)) \quad \text{(Eq. S20)}$$

$$R_D = 0.008 * Nitrifier * 1.0/(1.0 + [DOC])/(1.0 + F_\theta) \quad \text{(Eq. S21)}$$

Where *[DOC]* is dissolved organic carbon content (kg C/ha), F_θ is a soil moisture factor, and *Nitrifier* is biomass of nitrifier.

Net increase in nitrifier biomass:

$$dNitrifier/dt = (R_G - R_D) * Nitrifier * F_{Tmp} * F_\theta \quad \text{(Eq. S22)}$$

Nitrification rate:

$$N^{N_2O} = 0.005 * [NH_4^+] * Nitrifier * pH \quad \text{(Eq. S23)}$$

Where $[NH_4^+]$ is concentration of ammonium (kg N/ha) and *pH* is the soil pH.

Soil moisture factor in nitrification

$$F_\theta = 0.8 + 0.21 * (1.0 - WFPS) \qquad WFPS > 0.05 \quad \text{(Eq. S24)}$$

$$F_\theta = 0.0 \qquad WFPS \le 0.05 \quad \text{(Eq. S25)}$$

Where *WFPS* is the soil water content in water filled porosity.

Soil temperature factor in nitrification.

$$F_{Tmp} = 3.503^{((60-T)/25.78)} * e^{(3.503*(T-34.22)/25.78)} \quad \text{(Eq. S26)}$$

Where *T* is the soil temperature.

N_2O production through nitrification:

$$N_2O_N = 0.0024 * N^{N_2O} \quad \text{(Eq. S27)}$$

Denitrification process

In the DNDC model, denitrification process is a series of microbe-mediated reactions that sequentially reduce NO_3^- to NO_2^-, NO, N_2O, and finally to N_2. Denitrification rate is a function of denitrifiers, DOC, CO_2, N concentration, temperature, and pH in soils [32].

Relative growth rates of NO_x denitrifiers is simulated using:

$$R_{NO_x} = R_{NO_x,max} * ([DOC]/(K_C + [DOC])) * ([NO_x]/(K_N + [NO_x])) \quad \text{(Eq. S28)}$$

$$R_{DN} = F_{Tmp} * (R_{NO_3} * F_{pH-NO_3} + R_{NO_2} * F_{pH-NO_2} + R_{NO} * F_{pH-NO} + R_{N_2O} * F_{pH-N_2O}) \text{(Eq. S29)}$$

$$(dDenitrifier/dt)_g = R_{DN} * Denitrifier \qquad \text{(Eq. S30)}$$

Where $R_{NO_x,max}$ is the maximum growth rate of NO_3^-, NO_2^-, NO, or N_2O denitrifiers. *[DOC]* is dissolved organic carbon content (kg C/ha). *[NOx]* is concentration of NO_3^-, NO_2^-, NO, or N_2O in soil water (kg N/ha). K_c is half-saturation value of soluble C in the Monod model (kg C/m³ soil water). K_N is half-saturation value of NO_3^-, NO_2^-, NO or N_2O in the Monod model (kg N/m³ soil water). F_{Tmp} is a temperature factor. F_{pH-NO_3} , F_{pH-NO_2} , F_{pH-NO} and F_{pH-N_2O} is soil pH factors, and *Denitrifier* is biomass of denitrifier.

Relative death rates of denitrifiers:

$$(dDenitrifier/dt)_d = M_C * Y_C * Denitrifier \qquad \text{(Eq. S31)}$$

Where M_c is maintenance coefficient of C (kg C/kg C/ha) and Y_c is maximum growth yield on soluble carbon (kg C/kg C).

Consumption of DOC and CO_2 production through denitrification:

$$dC_{con}/dt = (R_{DN}/Y_C + M_C) * Denitrifier \qquad \text{(Eq. S32)}$$

$$d_{CO_2}/dt = dC_{con}/dt - dDenitrifier/dt \qquad \text{(Eq. S33)}$$

Consumption of NO_x through denitrification:

$$d(NO_3)/dt = (R_{NO_3}/Y_{NO_3} + M_{NO_3} * [NO_3]/[N]) * Denitrifier * F_{pH-NO_3} * F_{Tmp} \qquad \text{(Eq. S34)}$$

$$d(NO_2)/dt = (R_{NO_2}/Y_{NO_2} + M_{NO_2} * [NO_2]/[N]) * Denitrifier * F_{pH-NO_2} * F_{Tmp} \qquad \text{(Eq. S35)}$$

$$d(NO)/dt = (R_{NO}/Y_{NO} + M_{NO} * [NO]/[N]) * Denitrifier * F_{pH-NO} * F_{Tmp} \qquad \text{(Eq. S36)}$$

$$d(N_2O)/dt = (R_{N_2O}/Y_{N_2O} + M_{N_2O} * [N_2O]/[N]) * Denitrifier * F_{pH-N_2O} * F_{Tmp} \qquad \text{(Eq. S37)}$$

Where Y_{NO3}, Y_{NO2}, Y_{NO}, *and* Y_{N2O} is the maximum growth yield on NO_3^-, NO_2^-, NO, or N_2O (kg C/kg N). M_{NO3}, M_{NO2}, M_{NO}, *and* M_{N2O} is the maintenance coefficient of NO_3^-, NO_2^-, NO, or N_2O (kg N/kg/ha), and *[N]* is the total nitrogen as the sum of NO_3^-, NO_2^-, NO, and N_2O (kg N/ha).

Assimilation of N during denitrification:

$$dN/dt = (dDenitrifier/dt)_g/(C/N)_{Denitrifier} \qquad \text{(Eq. S38)}$$

Where $(C/N)_{Denitrifier}$ is C/N ratio in denitrifiers.

Soil temperature factor in denitrification:

$$F_{Tmp} = 2.0^{(T-22.5)/10.0} \qquad T \le 60.0 \qquad \text{(Eq. S39)}$$

$$F_{Tmp} = 0.0 \qquad T > 60.0 \qquad \text{(Eq. S40)}$$

Where *T* is the soil temperature.

Soil pH factor in denitrification:

$$F_{pH-NO_3} = 1 - 1/(1 + e^{((pH-4.25)/0.5)}) \qquad \text{(Eq. S41)}$$

$$F_{pH-NO_2} = F_{pH-NO} = 1 - 1/(1 + e^{((pH-5.25)/1)}) \qquad \text{(Eq. S42)}$$

$$F_{pH-N_2O} = 1 - 1/(1 + e^{((pH-6.25)/1.5)}) \qquad \text{(Eq. S43)}$$

Where *pH* is the soil pH.

3 The SWAT model

Nitrification process

The SWAT model treats nitrification as a function of soil NO_3^-, soil moisture and soil temperature [33]. We also list the equation here for considering the impact of soil pH on nitrification, which is used by Shrestha et al. [34] and Wagena et al. [35]. Therefore, the equation for nitrification is as following (Eq.S44):

$$N^{N_2O} = F_{NH_4} * K_2 * F_\theta * F_{Tmp} * F_{pH} \quad \text{(Eq. S44)}$$

Where N^{N_2O} is N_2O flux from nitrification (g N ha^{-1} d^{-1}), K_2 is the fraction of nitrified N lost as N_2O. F_{NH_4} is the rate of nitrification. F_θ , F_{Tmp} , and F_{pH} is the effect of soil moisture, temperature, and soil pH on nitrification, respectively.

The rate of nitrification:

$$F_{NH_4} = \frac{f_{nit}}{f_{nit}+f_{vol}} * N_{nitvol} \qquad \text{(Eq. S45)}$$

Where f_{nit} and f_{vol} are the fractions of N lost to nitrification and volatilization. N_{nitvol} (g Nha^{-1} d^{-1}) is the amount of ammonium converted via nitrification and volatilization.

The effect of soil moisture (F_θ) on nitrification:

$$F_\theta = \frac{SW_{ly}-WP_{ly}}{0.25*(FC_{ly}-WP_{ly})} \qquad if \quad SW_{ly} < 0.25 * FC_{ly} - 0.75 * WP_{ly} \qquad \text{(Eq. S46)}$$

$$F_\theta = 1.0 \quad if \quad SW_{ly} \geq 0.25 * FC_{ly} - 0.75 * WP_{ly} \qquad \text{(Eq. S47)}$$

Where SW_{ly} is soil water content (mm), WP_{ly} is the amount of water held in the soil at the wilting point water content (mm), and FC_{ly} is amount of water held in the soil layer at field capacity water content (mm).

The effect of soil temperature (F_{Tmp}) on nitrification is provided by the following factor:

$$F_{Tmp} = 0.41 * \frac{SoilTem-5}{10} \quad \text{if } SoilTem > 5 \qquad \text{(Eq. S48)}$$

The effect of soil pH (F_{pH}) on nitrification is provided by the following factor:

$$F_{pH} = 0.56 + \frac{arctan(\pi*0.45*(-5+soilpH))}{\pi} \qquad \text{(Eq. S49)}$$

Denitrification process

The SWAT model determines the amount of nitrate lost to denitrification with the equation (Eq. S50 and Eq. S51) [33]:

$$D_t = NO3_{ly} * (1 - exp(-\beta_{denit} * \gamma_{tmp,ly} * orgC_{ly})) \qquad if \gamma_{sw,ly} \geq \gamma_{sw,thr} \text{ (Eq. S50)}$$

$$N_{denit,ly} = 0.0 \qquad if \gamma_{sw,ly} < \gamma_{sw,thr} \quad \text{(Eq. S51)}$$

where D_t is the amount of nitrogen lost to denitrification (kg N/ha). $NO3_{ly}$ is the amount of nitrate in layer ly (kg N/ha). β_{denit} is the rate coefficient for denitrification. $\gamma_{tmp,ly}$ is the nutrient cycling temperature factor for layer ly. $\gamma_{sw,ly}$ is the nutrient cycling water factor for layer ly. $orgC_{ly}$ is the amount of organic carbon in the layer (%), and $\gamma_{sw,thr}$ is the threshold value of nutrient cycling water factor for denitrification to occur.

The effect of nutrient cycling temperature factor on denitrification:

$$\gamma_{tmp,ly} = Max\left[\left(0.9 * \frac{SoilTemp}{SoilTemp+e^{(9.93-0.312*SoilTemp)}} + 0.1\right), 0.1\right] \qquad \text{(Eq. S52)}$$

The effect of nutrient cycling water factor on denitrification:

$$\gamma_{sw,ly} = \frac{SW_{ly}}{FC_{ly}} \qquad \text{(Eq. S53)}$$

Where SW_{ly} is soil water content (mm) and FC_{ly} is amount of water held in the soil layer at field capacity water content (mm).

Wagena et al. [35] developed equations for the impact of soil pH on denitrification:

$$Fd(pH) = \begin{cases} 0.001 & for \quad pH \leq 3.5 \\ \frac{pH-3.5}{3} & for \quad 3.5 < pH < 6.5 \\ 1 & for \quad pH \geq 6.5 \end{cases} \qquad \text{(Eq. S54)}$$

Partitioning N_2O from N_2

For partitioning N_2O from gases of denitrification, Wagena et al. [35] used the same equations as Parton et al. [29] developed for the DAYCENT model (Eq.S12), and further included the effect of soil pH ($Fr(pH)$) for the ratio N_2O/N_2:

$$Fr(pH) = \frac{1}{1470 * e^{-1.1*pH}} \qquad \text{(Eq. S55)}$$

R codes used to plot and visualize the differences of the representation of each environmental factors on N_2O can be found in the following link: *https://github.com/snailslowrun/N2O/blob/main/comparison.R*

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