Development of the N$_2$O submodel of Biome-BGCMuSo 6.1 (beta32 and afterwards)

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Introduction

Biome-BGCMuSo v6.1 beta 31 (and all previous versions since version 5) uses a simple estimation of denitrification related N_2O gas flux based on the calculated denitrification rate (expressed in $kgN/m^2/day$). As the first step, denitrification is calculated followig this formula:

$$DN = D \cdot Rs \cdot [NO_3^-] \cdot SWC/SWC_s$$

where $[NO_3^-]$ is the amount of nitrate in the given soil layer ($kgN/m^2/layer$), D is the denitrification rate per gC of total soil respiration (proposed value is 0.05 gC^{-1}), Rs is soil heterotrophic respiration ($gC/m^2/day$), SWC is soil water contenr (m^3/m^3), and SWC_s is the saturated SWC.

Based on DN the N_2O gas flux is calculated as:

$$F_{N_2O,denitrif} = 1 / (1+0.16 \cdot WFPS) \cdot DN$$

where WFPS is the water filled pore space (estimated as SWC/SWC_s).

Problem

During the testing phase of the model it was found that there the total N_2O flux is overestimated by the model. The primary cause of the problem is the overestimation of the denitrificaiton related N_2O flux that is caused by the improper calculation of $F_{N_2O,denitrify}$. Here we propose an alternative formulae for the partitioning of N gas between N_2 and N_2O following the method of Parton et al. (1996) and Wagena et al. (2017).

Proposed new method

The following equation is used to calculate the ratio of N_2 and N_2O that is generated during denitrification:

$$R_{N2/N2O}=min[F_r(NO_3) , F_r(CO_2)] \cdot F_r(WFPS) \cdot F_r(pH)$$

where $R_{N2/N2O}$ is the ratio of N_2 and N_2O gas (both expressed as N equivalent mass), $F_r(NO_3)$ represents the effect of NO_3^- availability, $F_r(CO_2)$ is the modifier due to total soil respiration (proxy for microbial activity), $F_r(WFPS)$ shows the effect of SWC, and $F_r(pH)$ is included to represent the effect of soil pH (this latter was not included in Parton et al., 1996). Importance of pH is highlighted in Wang et al. (2017).

It is important to note that the equations presented in Wagena et al. (2017) are incorrect. The exact formulae of the equations is much better described in Parton et al. (1996) though their Fig. 5 also contains an error (equation describing the $F_r(NO_3)$ has a bracket problem). For clarity, here we provide explicit equations that are error-free according to our best knowledge.

The equation for $F_r(NO_3)$ (Parton et al., 1996):

$$F_r(NO_3) = (1 - (0.5+((atan(\pi \cdot 0.01 \cdot (NO_{3,ppm} - 190))) / \pi))) \cdot 25$$

where $NO_{3,ppm}$ is the nitrate content of the soil expressed in $\mu gN\ g^{-1}$ (=ppm). Note that for the calculation on $NO_{3,ppm}$ the soil's nitrate content has to be recalculated using the bulk density. Note also that the atan function is supposed to expect radians. The graphical representation of the equation is as follows:
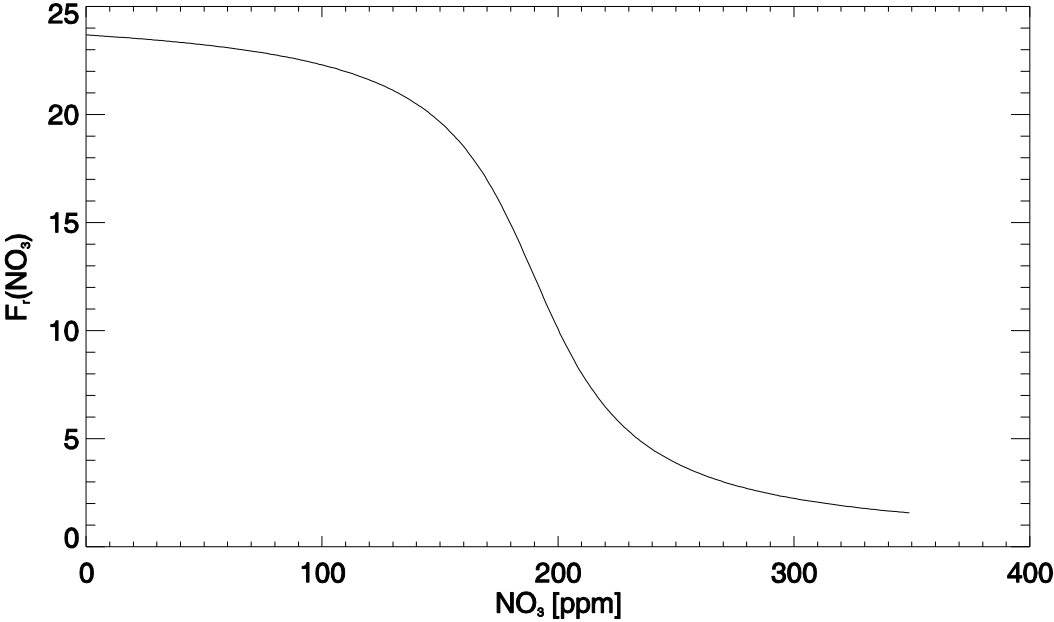
The equation for Rs (Parton et al., 1996):

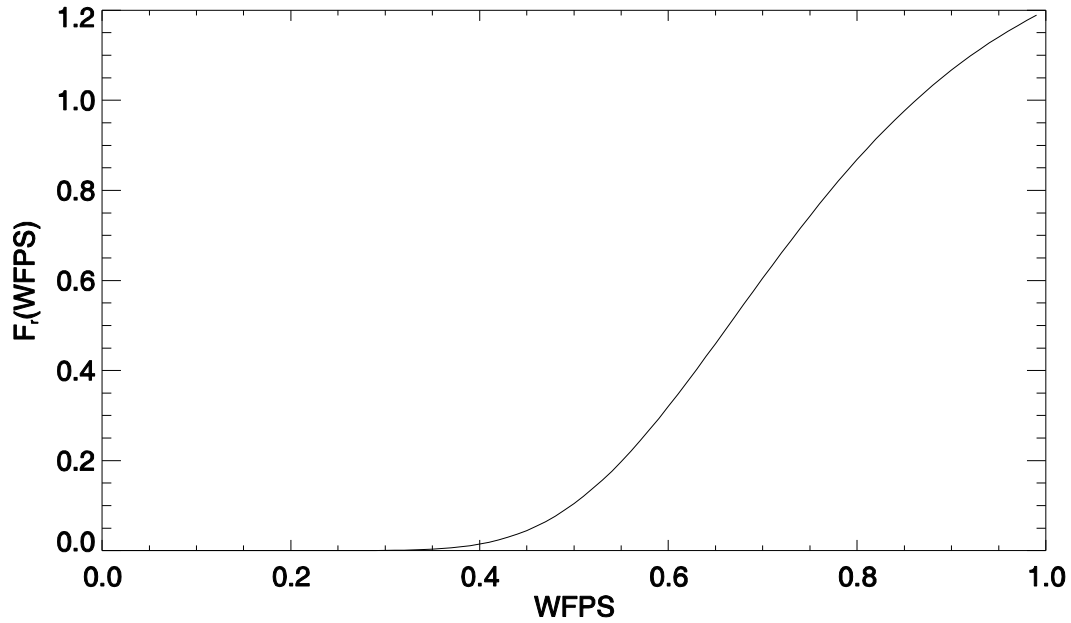$$F_r(CO_2) = 13 + ((30.78 \cdot atan(\pi \cdot 0.07 \cdot (R_{s,tot}-13))) / \pi)$$

where $R_{s,tot}$ is total soil respiration (heterotrophic component only; not only the soil respiration of the given soil layer!) expressed in $kgC\ ha^{-1}\ day^{-1}$. The graphical representation is:
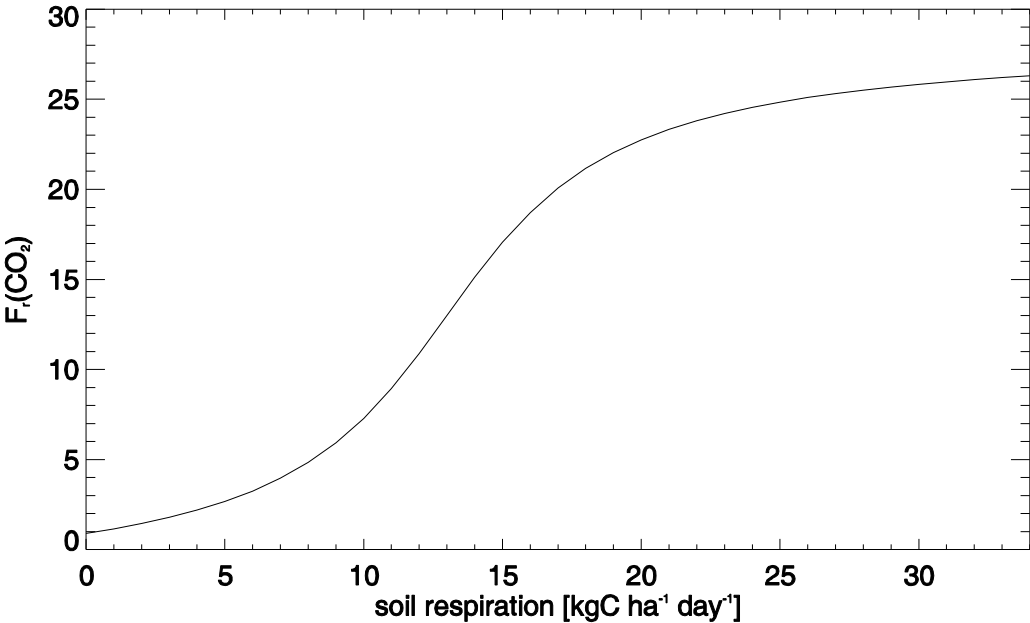
Next one is the equation for the WFPS effect on the ratio (Parton et al., 1996):

$$F_r(WFPS) = 1.4 / (13\wedge(17 / (13\wedge(2.2 \cdot WFPS))))$$

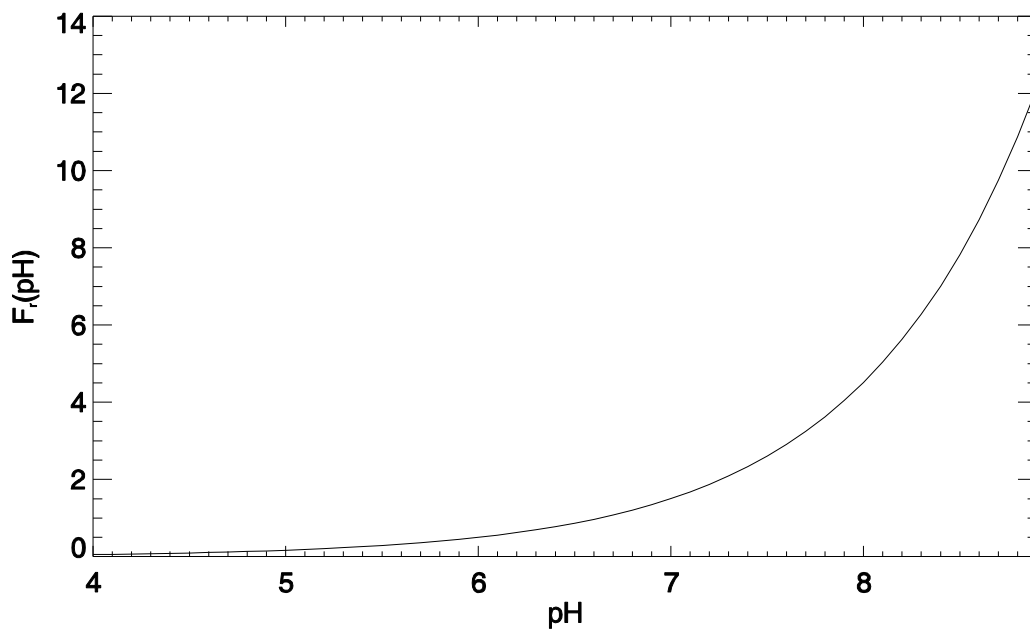The graphical form is the following:

The last equation addresses the effect of soil pH on the ratio (Wagena et al., 2017):

$$F_r(pH) = 1 / (1470 \cdot \exp(-1.1 \cdot pH))$$

The graphical form of the equation is:

After the calculations the final ratio is used to calculate denitrification related N2O flux from the amount of denitrification using this formula:

$$F_{N_2O,denitrif} = DN / (1 + R_{N2/N2O})$$

It is highly relevant to check the unit of the input data. Also, though it seems logical to use the given soil layer's soil respiration for the calculations THIS IS NOT THE CASE! The total (heterotrophic) soil respiration is needed in the scaling.

Application

We tested the modified ratio calculation method using 4 years of data from a simulation performed for Martonvásár. The following figure shows the original N2O flux emission caused by denitrification (black line), and the modified method (red line):
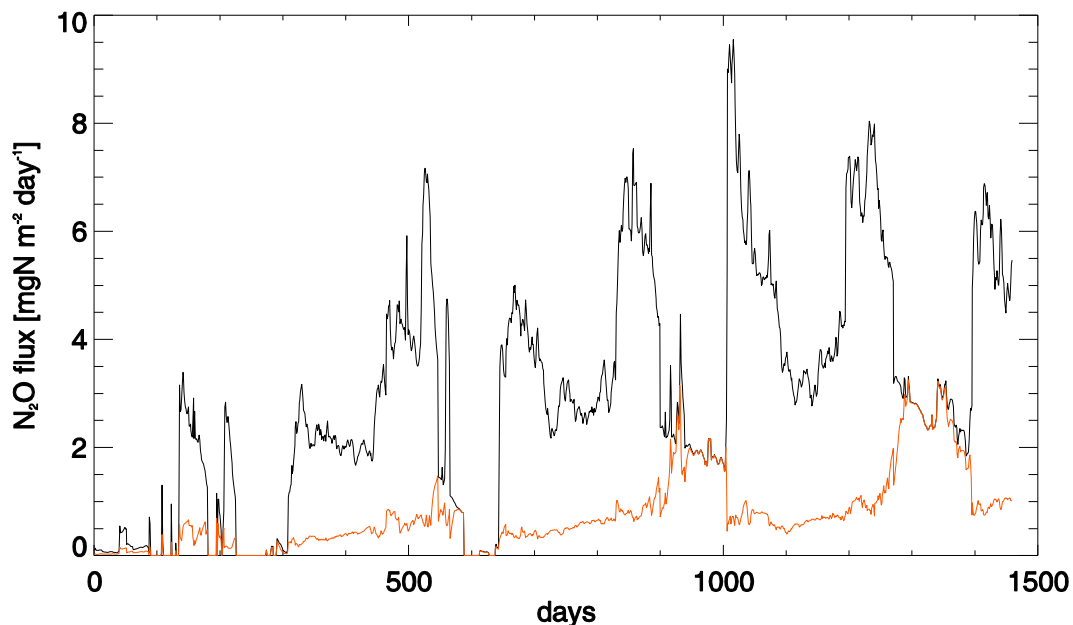
According to the figure the N2O fluxes are consideably smaller than in the original method. The magnitude of the fluxes is similar to those presented in the literature (Li et al., 2005; Haszpra et al., 2018).

Some further comments

The presented equations do not use information about the soil texture though it is proposed by e.g. Del Grosso et al. (2000) that soil texture strongly affects the calculated $R_{N2/N2O}$ (see Fig. 7 in Del Grosso et al., 2000).To resolve this issue we propose to include a parameter in the soil file that can act as a multiplier for the calculated $R_{N2/N2O}$. This multiplier can be set as texture –specific parameter during the construction of the soil files.

Some comments 1.

Alternative formulae for WFPS calculation (Wu et al., 2015):

WFPS is estimated as (Franzluebbers, 1999; Linn and Doran, 1984):

$$WFPS = \frac{\theta}{1 - \dfrac{\rho_d}{\rho_s}} \tag{7}$$

where ρ_d is the soil bulk density (g cm^{-3}), ρ_s is the particle density, typically around 2.65 g cm^{-3}, and θ is the volumetric water content (%).
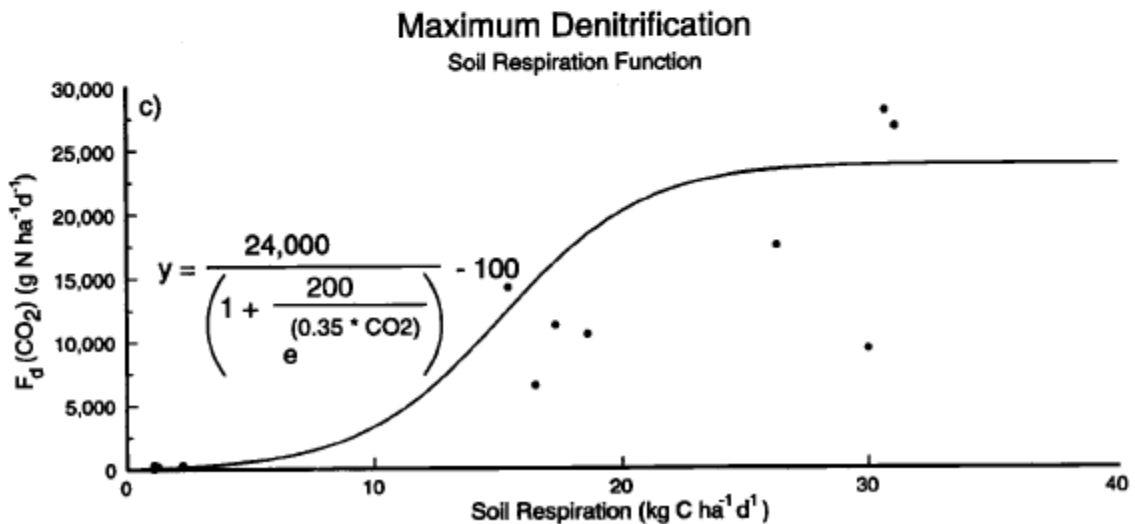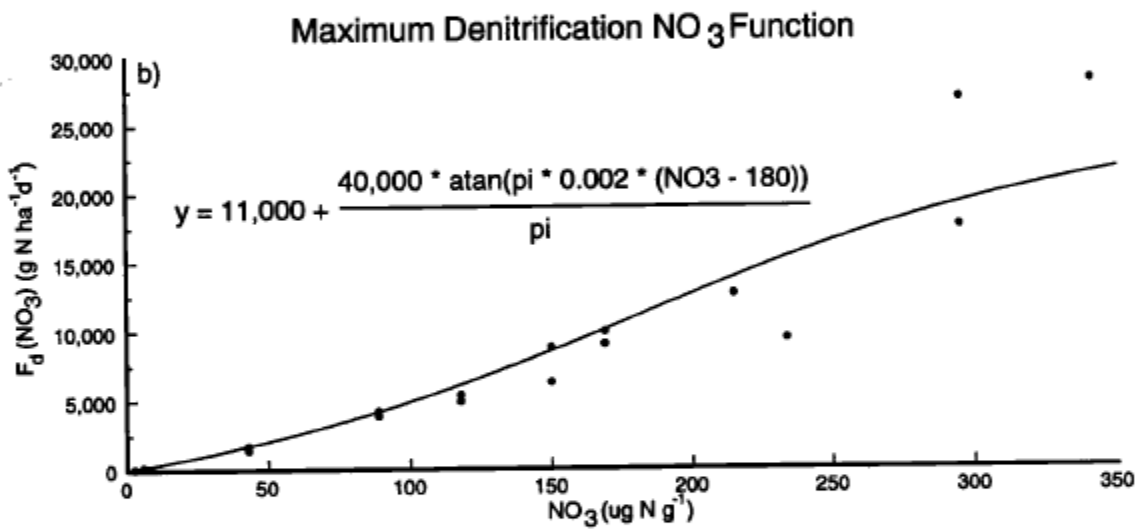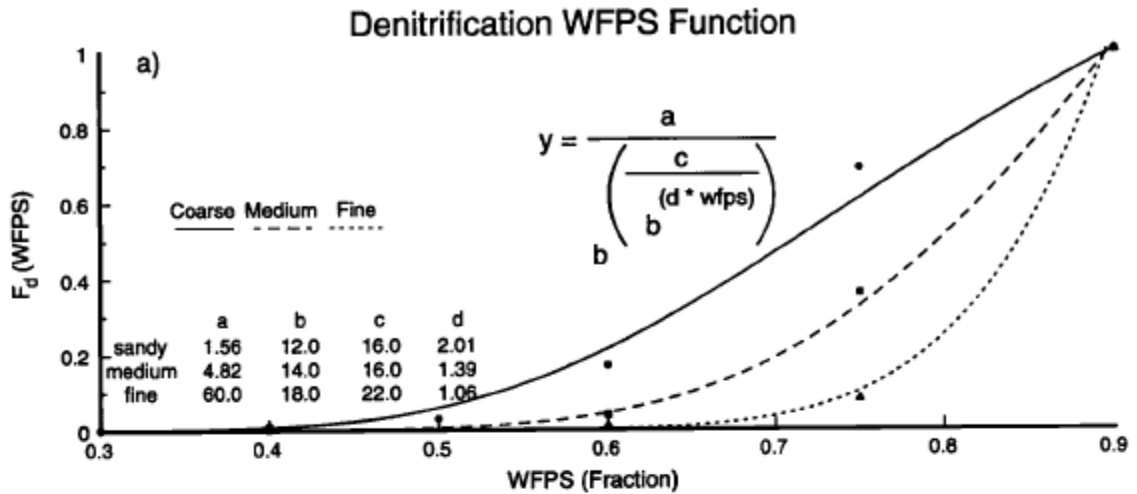
Some comments 2.

Alternative equations for the denitrification calculations are presented below. For simplicity, here we used screen shots from the Parton et al. (1996) and the Wagena et al. (2017) papers.

Note that the units are typically the same as presented above so it is relatively straightforward to implement those equations.

quantify denitrification-derived N$_2$ and N$_2$O. We developed a general model for total denitrification N(N$_2$+N$_2$O) gas fluxes (D$_t$ in g N ha^{-1} d^{-1}) as a function of soil heterotrophic respiration rate (index of carbon availability), soil NO$_3$ level, and soil WFPS using (2).

$$D_t = \min(F_d(NO_3), F_d(CO_2)) \; F_d(WFPS) \tag{2}$$

where F$_d$(NO$_3$) (see Figure 3b) is the maximum total N gas flux (g N ha^{-1} d^{-1}) for a given soil NO$_3$ level (assuming high respiration rates), F$_d$(CO$_2$) (see Figure 3c) is the maximum total N gas flux for a given soil respiration rate (assuming high NO$_3$ levels), and F$_d$(WFPS) (see Figure 3a) is the effect of WFPS on the

Denitrification WFPS Function

a)

F_d (WFPS)

Coarse Medium Fine

$$y = \dfrac{a}{b^{\left(\dfrac{c}{b^{(d\,*\,wfps)}}\right)}}$$

	a	b	c	d
sandy	1.56	12.0	16.0	2.01
medium	4.82	14.0	16.0	1.39
fine	60.0	18.0	22.0	1.06

WFPS (Fraction)

Maximum Denitrification NO$_3$ Function

b)

F_d (NO$_3$) (g N ha^{-1} d^{-1})

$$y = 11{,}000 + \dfrac{40{,}000 * atan(pi * 0.002 * (NO3 - 180))}{pi}$$

NO$_3$ (ug N g^{-1})

Maximum Denitrification
Soil Respiration Function

c)

F_d (CO$_2$) (g N ha^{-1} d^{-1})

$$y = \dfrac{24{,}000}{\left(1 + \dfrac{200}{e^{(0.35\,*\,CO2)}}\right)} - 100$$

Soil Respiration (kg C ha^{-1} d^{-1})

Figure 3. The effect of (a) water-filled pore space, (b) soil NO$_3$ level, and (c) soil respiration on total denitrification (N$_2$O + N$_2$) N gas flux. The curves were fit to the observed data presented in Figures 3a-3c [*Weier et al.*, 1993].

The total denitrification flux from Parton et al. (1996) and Mosier et al. (2002) is:

$$D_{Ntotal} = \min[Fd(NO_3), Fd(C)] * Fd(\theta) * Fd(T) * Fd(pH) \qquad (1)$$

where D_{Ntotal} is the denitrification rate per unit area (production of $N_2 + N_2O$, g N ha^{-1} d^{-1}); $Fd(NO_3)$ is the maximum total N gas flux per unit area for a given soil NO_3^- level in g N ha^{-1} d^{-1} (assuming total soil C is not limiting); $Fd(C)$ is the maximum total N gas flux per unit area for a given total soil C level in g N ha^{-1} d^{-1} (assuming soil N is not limiting); and $Fd(\theta)$, $Fd(T)$, and $Fd(pH)$ are functions that represent the effects of soil moisture, soil temperature, and pH on N gas flux, respectively. While the functional form of these relationships can differ to some extent, Parton et al. (1996) and Weier

Note that Wagena et al. (2017) uses the very same equations that Parton et al. (1996) but they propose to use two additional multipliers representing soil temperature and pH.

The soil temperature effect function, Fd(T), was derived from Seligman and Keulenv (1981):

$$Fd(T) = Max\left[\left(0.9 * \frac{Soil\ Temp}{Soil\ Temp + \exp(9.93 - 0.312 * Soil\ Temp)} + 0.1\right), 0.1\right]$$

$$(5)$$
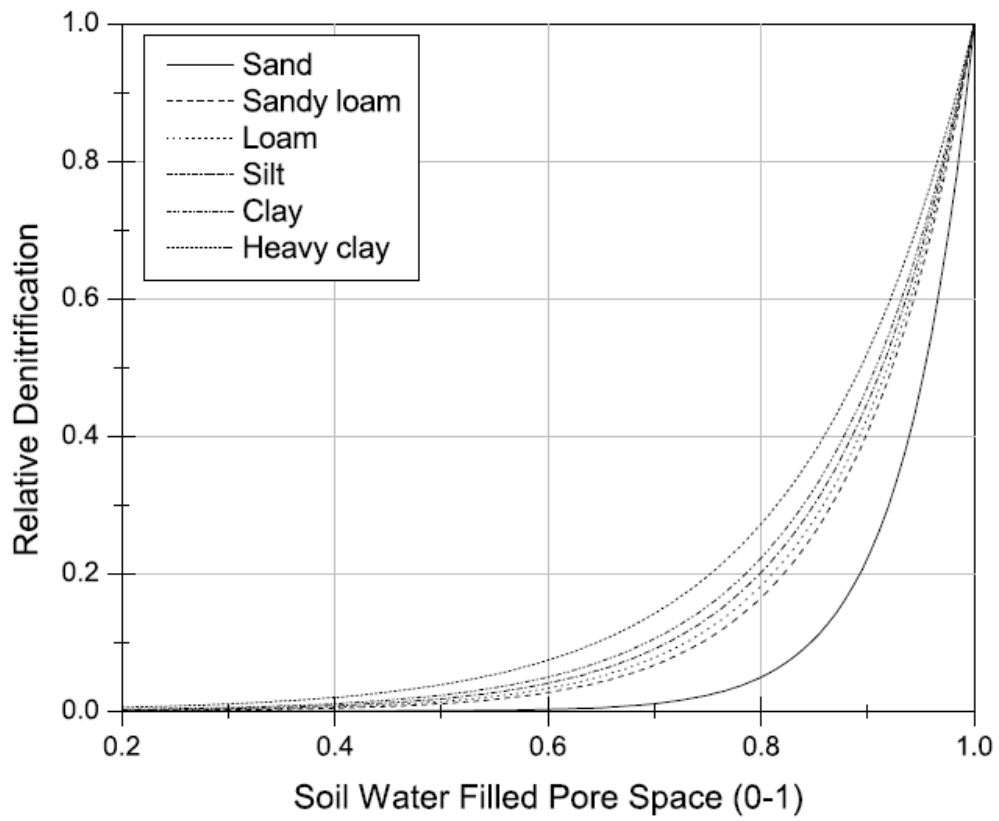
The pH function, Fd(pH), was developed from Simek and Cooper (2002):

$$Fd(pH) = \begin{cases} 0.001 & for\ pH \leq 3.5 \\ \dfrac{pH - 3.5}{3} & for\ 3.5 < pH < 6.5 \\ 1 & for\ pH \geq 6.5 \end{cases} \qquad (6)$$

Some comments 3.

Li et al. (2005) proposes this function:

Figure 1. Impact of soil water filled pore space on denitrification for different texture soils, used in WNMM gas module.

References

DelGrosso, S.J., Parton, W.J., Mosier, A.R., Ojima, D.S., Kulmala, A.E., Phongpan, S., 2000. General model for N_2O and N_2 gas emissions from soils when comparing observed and gas emission rates from irrigated field soils used for model testing NO_2. Global Biogeochem. Cycles 14, 1045–1060.

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Wu, L., Rees, R.M., Tarsitano, D., Zhang, X., Jones, S.K., Whitmore, A.P., 2015. Simulation of nitrous oxide emissions at field scale using the SPACSYS model. Sci. Total Environ. 530–531, 76–86. DOI:j.scitotenv.2015.05.064

Appendix

IDL subroutine for testing purposes

```
pro denitri_N2O_part, in_NO3, in_soilresp, in_WFPS, in_pH, out_R

; AIM: denitrification related gas flux partitioning
; calculating the ratio of N2/N2O during denitrification

; NO3 concentration unit: ug/g = ppm!!!!
; soil respiration unit: kgC/ha/day !!!
; WFPS: 0....1

;NO3=findgen(350)
;soilresp=findgen(35)
;WFPS=findgen(100)/100.
;pH=findgen(70)/10.

; input for testing
if n_params() lt 1 then begin
NO3=30.
soilresp=2.85
WFPS=0.9
pH=6.6

endif else begin

NO3=in_NO3
soilresp=in_soilresp
WFPS=in_WFPS
pH=in_pH

endelse

; nitrate
FrNO3=(1.-(0.5+(( 1.*atan(!PI*0.01*(NO3-190.)))/!PI) ))*25.
;plot, NO3, FrNO3

FrC=13.+( (30.78*atan (!PI*0.07*(soilresp-13.))    )/!PI  )
;plot, soilresp, FrC

FrWFPS=1.4/(13.^  (17./(13.^(2.2*WFPS)))  )
;plot, WFPS, FrWFPS

FrpH=1./(  1470.* exp(-1.1*pH))
;plot, pH, FrpH

; N2/N2O ratio:
R=min([FrNO3,FrC])*FrWFPS*FrpH
if n_params() lt 1 then begin
print, 'N2/N2O ratio:', R
endif
out_R=R
end
```