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MDPI

Review

A review of on-going advancements in Soil and Water Assessment Tool (SWAT) for nitrous oxide (N_2O) modeling

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Supplementary information

SWAT conceptualizes organic and inorganic pools of nitrogen in soil, with three forms in the organic and two forms in the inorganic pool [1]. Fresh organic nitrogen (plant residues and microbial biomass), active and stable organic pools related to soil humus (depending upon the availability of substrates for mineralization) represent three forms of organic pools. The inorganic (mineral) pool includes ammonium (NH_4^+) and nitrate (NO_3^-) forms of nitrogen. To initialize the concentration of nitrogen levels in soil, SWAT modelers can specify the nitrate and organic N in humic substance in all soil layers or such concentrations can be defined automatically by SWAT using a depth relationship as:

$$NO_{3conc,z} = 7 * \exp(-z/1000) \qquad \text{(S1)}$$

where, NO_{3conc} is the nitrate concentration at a given depth (ppm) and z is the depth of soil from the surface.

Similarly, organic N is estimated using the assumed C:N ratio as:

$$OrgN_{hum,ly} = 10^4 * (OrgC_{ly}/14) \qquad \text{(S2)}$$

where, $OrgN$ is the concentration (ppm) of organic nitrogen in humic material in each layer (ly) and $OrgC$ is the amount of organic carbon in that layer (%).

The active and stable pools of organic N are estimated using a fraction value of 0.02. The amount of nitrogen in fresh organic pool is assumed as 0.15% of the initial soil surface residue for top 10 mm of soil and zero for underlying soil layers. The amount of ammonium is initialized to 0 ppm for each soil layer. The concentrations of nitrogen are then converted to mass by multiplying with bulk density and depth of the soil layer.

In SWAT, mineralization or immobilization occurs in soil when soil temperature exceeds 0°C and C:N conditions of soil organic matter are met [2]. Mineralization means breakdown of complex and plant unavailable forms of nitrogen to available forms of nitrogen (i.e. ammonium and nitrate forms) while immobilization means the reverse. For a C:N ratio >30, immobilization occurs, for <20, mineralization occurs and between 20-30, an equilibrium between both immobilization and mineralization takes place [1]. Two factors influencing mineralization (i.e. nutrient cycling temperature ($\gamma_{tmp,ly}$) and nutrient cycling water content ($\gamma_{sw,ly}$)) are estimated in SWAT as:

$$\gamma_{tmp,ly} = 0.9 * T_{soil,ly} / (T_{soil,ly} + \exp(9.93 - 0.312 * T_{soil,ly})) + 0.1 \qquad \text{(S3)}$$

$$\gamma_{sw,ly} = SW_{ly} / FC_{ly} \qquad \text{(S4)}$$

where, T_{soil} is the temperature (in °C), SW is the water content of soil and FC is the field capacity of each layer (ly). Nutrient cycling temperature is never allowed to fall below 0.1 and nutrient cycling water content is not allowed to fall below 0.05.

Free movement of nitrogen within different pools of humus fractions of SWAT is estimated using β_{trans} (rate constant: 10^{-5}), $orgN$ (N in active organic pool), $orgN_{sta}$ (N in stable organic pool) and fr_{actN} (fraction of humic nitrogen in pool:0.02):

$$N_{trns,ly} = \beta_{trns} * orgN_{act,ly} * (1/fr_{actN} - 1) - orgN_{sta,ly} \qquad \text{(S5)}$$

Positive value of N_{trans} indicates nitrogen movement from active to stable pool and negative indicates the opposite. An addition of nitrate mineralization from active humus organic pool is calculated as a function of nutrient cycling temperature ($\gamma_{tmp,ly}$) and water ($\gamma_{sw,ly}$) in a soil layer (*ly*) and the amount of nitrogen in active organic pool ($orgN_{act}$) as:

$$N_{mina,ly} = \beta_{min} * (\gamma_{tmp,ly} * \gamma_{sw,ly})^{0.5} * orgN_{act,ly} \tag{S6}$$

where β_{min} is the rate coefficient for mineralization of humus active organic nutrients.

The residues are mineralized in the first soil layer, as controlled by a decay rate constant which is updated daily. The daily decay rate constant is estimated using a function of C:N and C:P (carbon: phosphorus) ratios, temperature and soil water content of the residue. The decay rate constant ($\delta_{ntr,ly}$) defines the fraction that has been decomposed in the residue and can be calculated as:

$$\delta_{ntr,ly} = \beta_{rsd} * \gamma_{ntr,ly} * (\gamma_{tmp,ly} * \gamma_{sw,ly})^{0.5} \tag{S7}$$

where β_{rsd} is the rate coefficient of mineralization of residue fresh organic nutrients and γ_{ntr} is the nutrient cycling residue composition factor, which are dependent on C:P and C:N ratios.

Mineralization (N_{minf}) and decomposition (N_{dec}) from the residue fresh organic pool are then calculated as:

$$N_{min,ly} = 0.8 * \delta_{ntr,ly} * orgN_{frsh,ly} \tag{S8}$$

$$N_{dec,ly} = 0.2 * \delta_{ntr,ly} * orgN_{frsh,ly} \tag{S9}$$

The decomposed nitrogen from fresh organic pool is added to the active organic pool and once initialized, nitrification and volatilization occurs in SWAT following methods of Reddy, *et al.* [3] and Godwin, *et al.* [4]. Nitrification in SWAT is a function of soil temperature and water content while volatilization is a function of soil depth, temperature and cation exchange capacity. Four coefficients are used in the algorithms defining nitrification and volatilization and these processes are activated when temperature of soil exceeds 5°C. The nitrification/volatilization temperature factor ($\eta_{tmp,ly}$) is calculated with respect to soil temperature ($T_{soil,ly}$) as:

$$\eta_{tmp,ly} = 0.41 * (T_{soil,ly} - 5)/10 \qquad \text{if} \quad T_{soil,ly} > 5 \tag{S10}$$

The nitrification soil water factor ($\eta_{sw,ly}$) is estimated as a function of soil water content on a given day (*SW*), amount of water held in soil at wilting point (*WP*) and field capacity (*FC*) in each layer (*ly*) as:

$$\eta_{sw,ly} = (SW_{ly} - WP_{ly})/(0.25*(FC_{ly} - WP_{ly})) \qquad \text{if} \quad SW_{ly} < 0.25*FC_{ly} - 0.75*WP_{ly} \tag{S11}$$

$$\eta_{sw,ly} = 1 \qquad \text{if} \quad SW_{ly} \geq 0.25*FC_{ly} - 0.75*WP_{ly} \tag{S12}$$

Similarly, the volatilization depth factor is calculated as:

$$\eta_{midz,ly} = 1 - Z_{mid,ly}/(Z_{mid,ly} + \exp(4.706 - 0.0305*Z_{mid,ly})) \tag{S13}$$

The impact of environmental factors on nitrification and ammonia volatilization in each layer is defined by the nitrification regulator and volatilization regulator, which are calculated as:

$$\eta_{nit,ly} = \eta_{tmp,ly} * \eta_{sw,ly} \tag{S14}$$

$$\eta_{vol,ly} = \eta_{tmp,ly} * \eta_{midz,ly} * \eta_{cec,ly} \tag{S15}$$

Similarly, SWAT determines the amount of nitrate lost through denitrification, as a function of rate coefficient of denitrification, nutrient cycling temperature and water factors, % organic carbon and threshold value of nutrient cycling water factor to start denitrification as:

$$N_{denit,ly} = NO_{3ly} * 1 - \exp(-\beta_{denit} * \gamma_{tmp,ly} * orgC_{ly}) \qquad \text{if} \ \gamma_{sw,ly} \geq \gamma_{sw,thr} \tag{S16}$$

$$N_{denit,ly} = 0 \qquad \text{if} \quad \gamma_{sw,ly} < \gamma_{sw,thr} \tag{S17}$$

References

1. Neitsch, S.L.; Arnold, J.G.; Kiniry, J.R.; Williams, J.R. *Soil and water assessment tool theoretical documentation version 2009*; Texas Water Resources Institute: 2011.
2. Seligman, N.; Keulen, H. 4.10 PAPRAN: A simulation model of annual pasture production limited by rainfall and nitrogen. *Simulation of nitrogen behaviour of soil-plant systems* **1980**, *192*.
3. Reddy, K.; Khaleel, R.; Overcash, M.; Westerman, P. A nonpoint source model for land areas receiving animal wastes: II. Ammonia volatilization. *Transactions of the ASAE* **1979**, *22*, 1398-1405.
4. Godwin, D.; Jones, C.; Ritchie, J.; Vlek, P.; Youngdahl, L. The water and nitrogen components of the CERES models. In Proceedings of Proceedings of the International Symposium on Minimum Data Set for Agrotechnology Transfer (ICRISAT; pp. 101-106.