Ch. 7 Mineral Nitrogen

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7 Mineral nitrogen

7.1 Introduction

In this chapter, we describe the processes related to mineral nitrogen, i.e. nitrate and ammonium. However, the organic and inorganic N-processes are closely related in the N-cycle as implemented in Daisy, Figure 7.1. Therefore, the gross mineralization, i.e., the transformation process from organic N to ammonium, is described in Chapter 9, while the plant uptake of nitrate and ammonium, as well as symbiotic N-fixation and conversion of mineral N to plant material, is described in Chapter 10.

Mineral N may be added to the system as fertilizer or through atmospheric deposition given with weather data (Chapter 2). Ammonium may volatilize from both mineral and organic fertilizer, but the potential volatilized fraction is specified by the user. Ammonium sorbs to clay, and the sorption process is included in the model. Ammonium may nitrify to nitrate, with some N lost as N_2O during this process. Leaching of ammonium may take place following the solute transport equations (Chapter 6) but it is generally negligible due to the sorption and transformation processes. Nitrate does not sorb and is thus much more prone to leaching (described by the solute transport equations), but it may also denitrify to N_2 and N_2O.

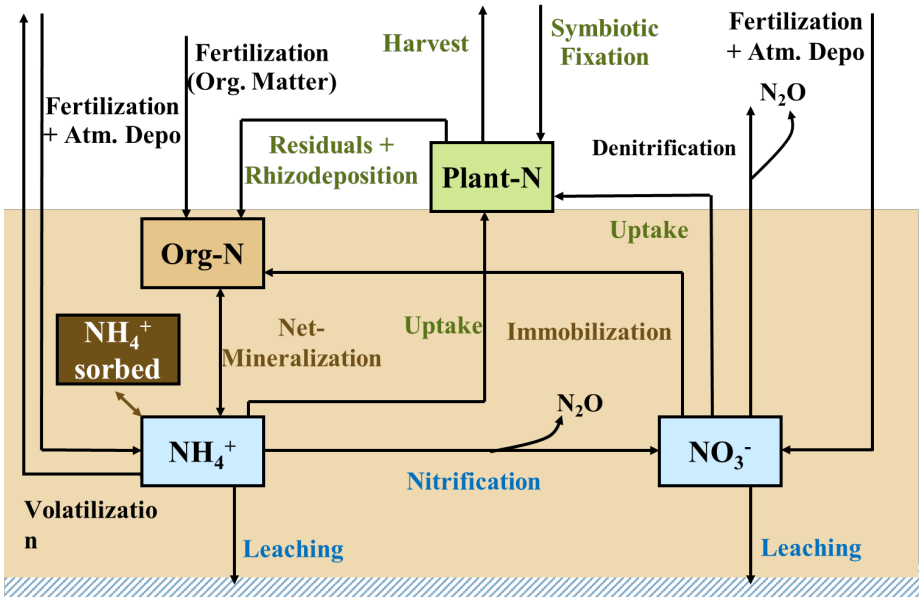

Figure 7.1. Nitrogen processes in Daisy.

7.2 Definitions of inorganic N-forms

Nitrate and ammonium are defined in Daisy as chemicals (Chapter 6). It means that, in principle, all the parameters available to describe a chemical can be used to describe the two compounds. They are defined in a hierarchical system, where “nutrient” is a sub-group of chemicals, “N” is a sub-group of “nutrient”, “MIN” is a sub-group of “N”, containing non-organic nitrogen, and finally “NH4” and "NO3” are the specific chemicals (NH_4^+-N and NO_3^--N) based on the sub-group “N”.

"nutrient" properties

The nutrient class provides chemicals in this group with the following properties:

(*canopy_dissipation_rate* 0 [h^{-1}])

(*canopy_washoff coefficient* 1 [])

(*decompose_rate* 0 [h^{-1}])

Thus, nutrients are not lost by dissipation on the canopy; if deposited on a canopy, they wash off the canopy with the first rain, and they do not decompose in the way described for pesticides. In principle, the group inherits the "*crop_uptake_reflection_factor*" with a default of 1 (no uptake) from the "base" definition of a chemical. However, nitrate and ammonium have their own uptake models, so this factor is only used to avoid that the two compounds are taken up "twice".

"NH4" properties

The "NH4" model for ammonium N allows definition of the adsorption model to use specification of an initial amount of NH_4^+-N in the soil [g cm^{-3}] and the diffusion coefficient for NH_4^+ (by default $1.8 \cdot 10^{-5}$ [cm^2 s^{-1}]).

It is possible to choose any of the adsorption models available in Daisy, but the default model is a linear adsorption model ("NH4"). Another model for ammonium sorption ("vS_S"), with a parameterization based on adsorption of K+ to illite, was default at least until year 2000 (it is not clear, when the default changed). Both models are described in section 7.4.

By default, an initial NH_4^+-N concentration in soil water of $0.5 \cdot 10^{-6}$ [g NH4-N cm^{-3}] is specified, as an assumption of no ammonium present would be erroneous due to contributions from deposition and mineralization.

"NO3" properties

The "NO3" model allows definition of an initial amount of NO_3^--N [g cm^{-3}] and a diffusion coefficient with a default value of $2 \cdot 10^{-5}$ [cm^2 s^{-1}]. By default, an initial NO_3^--N concentration of about half the amount allowed in drinking water is used for the soil water, $5.0 \cdot 10^{-6}$ [g NO_3-N cm^{-3}], as an assumption of no nitrate present would be erroneous. The initial value is about half to one third of the flow-weighted NO_3^-N concentration measured in the Danish monitoring program at 1 m's depth from 2004/5 – 2015/16 (Blicher-Mathiesen et al., 2023).

To obtain reasonable values of inorganic N-compounds in the soil, it is recommended to use a warm-up period for one's model. The initial values can be changed by the user.

7.3 Input of mineral nitrogen

7.3.1 Mineral fertilizer and volatilization

A mineral fertilizer is defined with a name, an NH_4^+-N-fraction (NH4_fraction []), and a volatilization fraction [-]. The amount that is not NH_4^+-N is expected to be NO_3^--N. When applied, the weight [kg N ha^{-1}] requires specification. Thus, the amount added in Daisy is not the amount of fertilizer, but only the amount of N added. Several mineral fertilizers have been defined in "fertilizer.dai" in the "lib"-

directory distributed with the model. A few of the entries in this file are shown below. The defined fertilizers do not have volatilization specified. The user has to add a line, e.g. (volatilization 0.05 []) to introduce volatilization of the ammonium fraction.

```
(defam NPK02 mineral
  (description "Various NPK fertilizers")
  (NH4_fraction 0.57 []))

(defam NP mineral
  (description "Typical NP or NPS fertilizer")
  (NH4_fraction 0.650 []))

(defam CalciumNitrate mineral
  (description "Kalksalpeter")
  (NH4_fraction 0.08 []))
```

Management operations are further described in Chapter 11. However, a typical application of a fertilizer at the surface can be specified as follows:

(wait_mm_dd 4 05) (fertilize (NP (weight 145 [kg N/ha]))) or

(wait (at 1987 4 4 1)) (fertilize (mineral (weight 100.0 [kg N/ha])
(NH4_fraction 0.5 [])))

The first example describes a date of application in any year, the fertilizer to be added, and the weight in kg N/ha. The second example describes a specific date and hour where a specified amount of mineral fertilizer with a specified NH_4^+-N-fraction is added.

7.3.2 Inorganic N in organic fertilizers

The description of organic fertilizers can be found in Chapter 9, but it should be noted that organic fertilizers may also contain inorganic N-compounds. First, the total N-content is defined as the N-fraction of dry matter, and then NH_4^+-N- and NO_3^-N- fractions are defined as part of the total N, with the assumption that the rest will be organic N.

7.3.3 Deposition

Deposition of NH_4^+-N and NO_3^--N is specified in the Daisy weather file and has already been mentioned in Section 2.2.5 and 3.5.3. Dry deposition is specified as kg NH_4-N ha^{-1} $year^{-1}$ and kg NO_3-N ha^{-1} $year^{-1}$ [or kg m^{-2} day^{-1}]. Wet deposition of the same two compounds is specified as a concentration, typically ppm [mg l^{-1}], in precipitation. The rates should be calculated based on measurements. Precipitation data is required to calculate the mass fluxes for the wet deposition, or – if mass fluxes are recorded, to convert the mass fluxes to concentrations. In Denmark, annual estimates are available from DCE (Institute for Environmental Science), Aarhus University. Examples of distribution of total N-deposition over space and time is shown in Figure 7.2. For shorter periods (a decade), constant

values may be adequate for a given site, but the total amount varies significantly across the country.

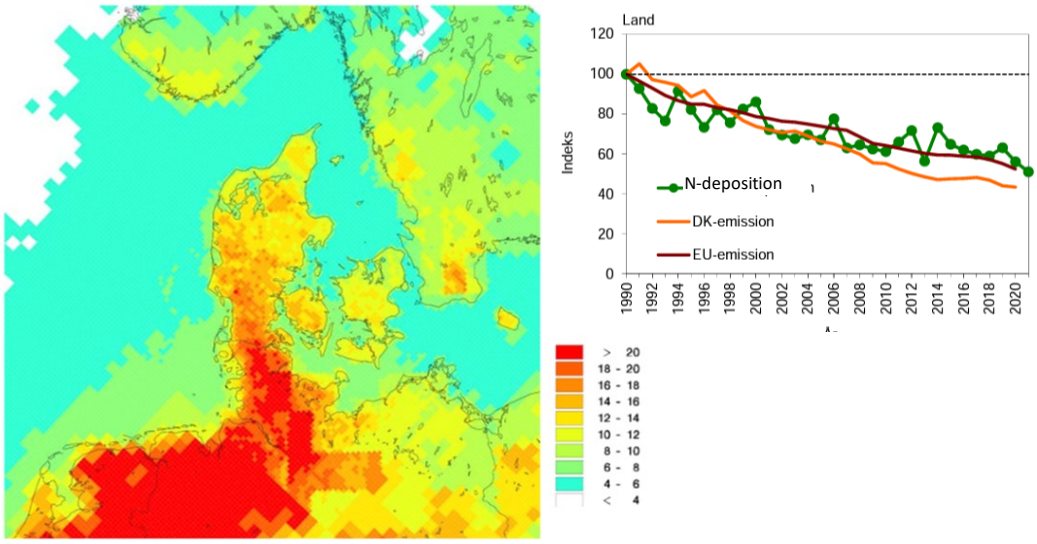

Figure 7.2. a) N-deposition in Denmark calculated for 2021 [kg N/ha], and b) development in deposition in Denmark over time, indexed to 1990, shown together with the emission in Denmark and EU (Ellermann et al., 2023).

7.4 Sorption of ammonium

Sorption of ammonium to clay

Ammonium sorbs to clay, and clay exists in different forms. Clay consists of tetrahedral layers based on SiO_2-building blocks and octahedral layers based on Aluminium, and the charge of the layers comes from substitution. If Si is substituted by Al, a negative charge is generated, and the same happens if Al is substituted by Fe2+, Mg2+, and so on. For illite, the three-layer components are held tightly together by potassium ions which fits perfectly into the octahedral layers. Other 3-layer clay minerals tend to have more water and higher distances between the clay units. Ammonium and potassium ions have the same size, so they can be substituted. Two-layer clay minerals have no potassium interlayer and usually low electrical charge. More information on clay minerals can be found in, among others, Blume et al. (2016) and Kumari and Mohan (2021).

Theory by Schouwenburg and Schuffelen (1963)

The theory in the original default model for ammonium sorption comes from a study of K+-sorption in illite (Schouwenburg and Schuffelen, 1963). In that study, they found that although free potassium can enter the interlayer space, the capacity is quite small. The capacity for sorption is about 10 times larger on the edges and more than 10 times higher on the planar sites compared to the interlayer space.

For illitic clay, Schouwenburg and Schuffelen (1963) described potassium-calcium exchange by eq.(7.1), using a double Langmuir isotherm, where interlayer adsorption is ignored:

$$\gamma_{K^+} = 0.4258\frac{2.21 \cdot R}{1 + 2.21 \cdot R} + 0.020\frac{102.3 \cdot R}{1 + 102.3 \cdot R} \quad (7.1)$$

γ_{K^+} = potassium adsorbed [m.e. g^{-1} (clay)] (m.e. = milli equivalents)

R = $C_{K^+}/(C_{Ca^{++}})^{1/2}$

C_{K^+} = concentration of potassium [mole l^{-1}]

$C_{Ca^{++}}$ = concentration of calcium [mole l^{-1}]

To make units fit, "1" must be [mole l^{-1}], the factors multiplied onto R in the equation must be [mole $l^{-1}]^{1/2}$, and the two factors in front of the fractions must be in [m.e. g^{-1} (clay)].

Potassium-ammonium exchange on a clay mineral may be quantitatively described as:

$$clay - K^+ + NH_4^+ = clay - NH_4^+ + K^+ \tag{7.2}$$

$$\frac{\gamma_{NH_4^+}}{\gamma_{K^+}} = K_{NH_4^+/K^+} \cdot \frac{C_{NH_4^+}}{C_{K^+}} \tag{7.3}$$

$\gamma_{NH_4^+}$ = ammonium adsorbed [m.e. g^{-1} (clay)]

γ_{K^+} = potassium adsorbed [m.e. g^{-1} (clay)]

$C_{NH_4^+}$ = concentration of ammonium [mole l^{-1}]

C_{K^+} = concentration of potassium [mole l^{-1}]

$K_{NH_4^+/K^+}$ = exchange coefficient

As $K_{NH_4^+/K^+}$ = 1, it is clear from eq.2 and 3, that K^+ and NH_4^+ behave similarly.

Assuming calcium to be the dominant divalent cation, and $C_{Ca^{++}}$ = 0.01 mole l^{-1}, eq. (7.1) can be re-written as

$$\gamma_{K^+} = 0.4258\frac{22.1 \cdot C_{K^+}}{1 + 22.1 \cdot C_{K^+}} + 0.020\frac{1023 \cdot C_{K^+}}{1 + 1023 \cdot C_{K^+}} \tag{7.4}$$

The factors multiplied onto C_{K^+} in the equation are now dimensionless.

By introducing the molar weight for ammonium-N, (14.0067 g mol^{-1} or $14 \cdot 10^{-3}$ g $mmol^{-1}$], the expression can be rewritten for ammonium as follows (eq. (7.5)):

$$\gamma_{M,NH_4^+} = \left[0.4258\frac{\frac{22.1}{14} \cdot C_{M,NH_4^+}}{1 + \frac{22.1}{14} \cdot C_{M,NH_4^+}} + 0.020\frac{\frac{1023}{14} \cdot C_{M,NH_4^+}}{1 + \frac{1023}{14} \cdot C_{M,NH_4^+}}\right] \cdot 14 \cdot 10^{-3}$$

where

γ_{M,NH_4^+} = NH_4^+-N adsorbed [kg N. kg^{-1} (clay)], and

C_{M,NH_4^+} = concentration of NH_4^+-N in soil solution [kg N m^{-3}].

Note the changed units.

vS_S_Styczen

By rearranging the fractions, equation (7.5) can be simplified to eq. (7.6):

$$\gamma_{M,NH_4^+} = \left[5.964 \cdot 10^{-3} \frac{C_{M,NH_4^+}}{0.6338 + C_{M,NH_4^+}} + 0.2801 \cdot 10^{-3} \frac{C_{M,NH_4^+}}{0.01369 + C_{M,NH_4^+}}\right]$$

Or

$$\gamma_{M,NH_4^+} = V_p \frac{C_{M,NH_4^+}}{K_p + C_{M,NH_4^+}} + V_e \frac{C_{M,NH_4^+}}{K_e + C_{M,NH_4^+}} \quad (7.7)$$

in which V_p and V_e [kg N. kg^{-1} (clay)] are the absorption capacity of the planer sites and edges of the clay, respectively, K_p and K_e [kg N m^{-3}] are the half-saturation constants of the planer sites and edges of the clay, respectively. V_p, K_p, V_e and K_e can be viewed as parameters depending on the exchange properties of the clay. In this parameterization (*vS_S_Styczen*), they have the values specified in eq. (7.6) and are hard-coded.

The relationships expressed by eq. (7.6) is shown in Figure 7.3 and Figure 7.4.

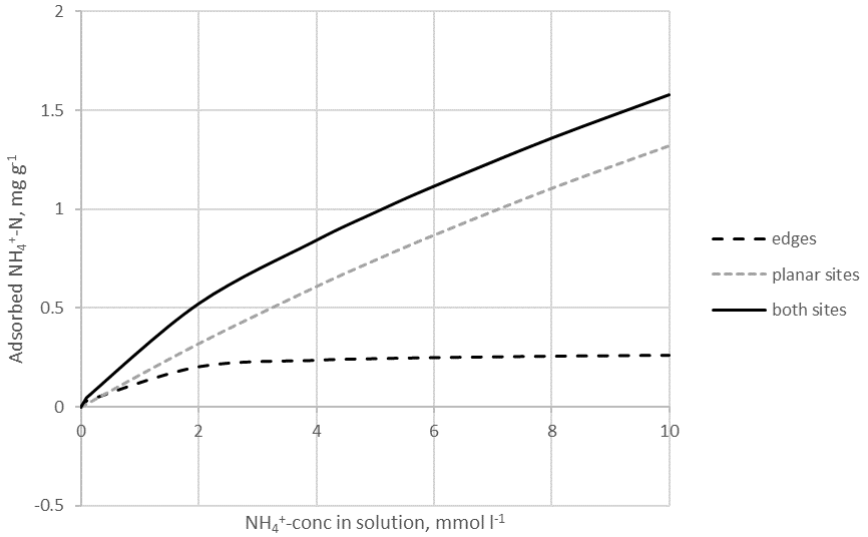

Figure 7.3. NH_4^+-N adsorption isotherms for various adsorption sites in the concentration range 0-10 mmol l^{-1}.

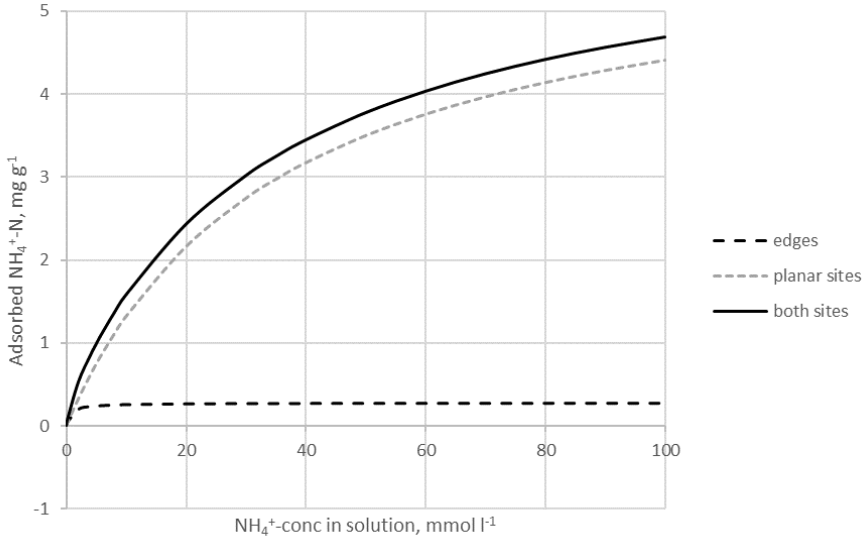

Figure 7.4. NH_4^+-N adsorption isotherms for various adsorption sites in the concentration range 0-100 mmol l^{-1}.

Calculated ammonium sorption in soil [kg N m^{-3} (soil)] then becomes:

$$A_{M,NH_4^+} = x_c \rho_b \left[\frac{V_p C_{M,NH_4^+}}{K_p + C_{M,NH_4^+}} + \frac{V_e C_{M,NH_4^+}}{K_e + C_{M,NH_4^+}} \right] \quad (7.8)$$

where A_{M,NH_4^+} is the absorbed NH_4^+, x_c is the clay content [ ], ρ_b is the bulk density [kg m^{-3}], and other parameters are defined earlier.

The total amount of NH_4^+ in the soil is the adsorbed amount plus the amount in soil solution: $\theta \cdot C_{am}$, where θ is soil water content and C_{am} is dissolved ammonium.

If soils are dominated by other clay minerals, it could be relevant to consider whether the default values should be changed, or a different sorption model applied. Particularly for two-layer minerals, the values could be very different.

This model does not include sorption to organic matter.

NB: The parameterization shown above is applied in the model vS_S_Styczen available from version 7.0.7. The earlier versions (vS_S_old and vS_S_Hansen) contained errors, resulting in too strong sorption of NH_4^+. The old parameterization and a test on the effect of the different parameterization on N dynamics are presented in appendix 7.1.

Linear sorption, the "NH4"-model

The linear sorption model for ammonium ($\gamma_{M,NH_4^+} = K \cdot C_{M,NH_4^+}$), which is presently implemented in Daisy as default, allows definition of a sorption value for clay (K_{clay}) and a sorption value for organic material (K_{OC}). It is built on the fact that in the range of ammonium concentrations typically found in the soil, the relationship between absorbed and dissolved ammonium is, in fact, close to linear. The initial concentration of NH_4^+ in the soil is $0.5 \cdot 10^{-6}$ [g NH_4-N cm^{-3}], or 0.036 [mmole l^{-1}]. Frequently found concentrations of NH_4^+ in arable soils are 0.2-4 mg l^{-1}, while the

total range is <0.1-16 mg l^{-1} according to Blume et al. (2016). The N-fraction is approximately 78 % of these values. Figure 7.5 shows the relationship between adsorbed NH_4^+-N and NH_4^+-N in solution from 0 to 3 mg l^{-1} calculated with the Schouwenburg and Schuffelen-model.

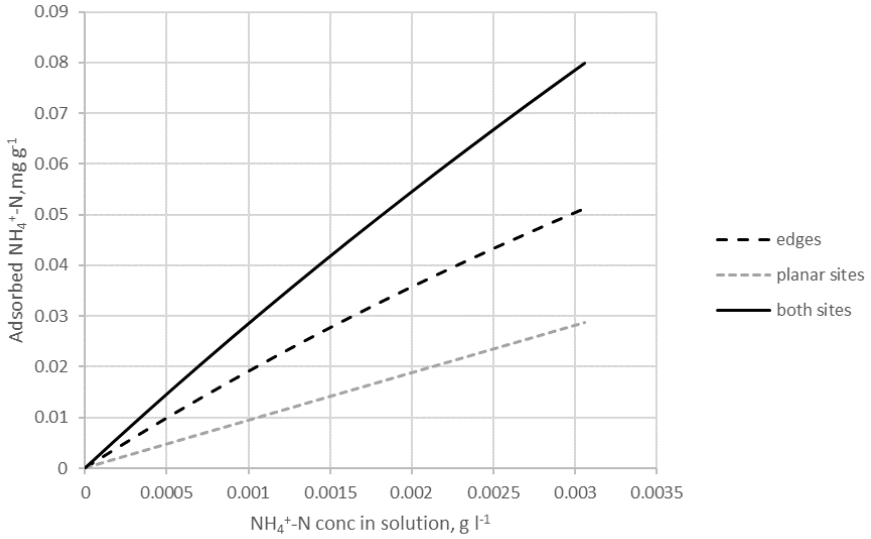

Figure 7.5. NH_4^+-N adsorption isotherms for various adsorption sites in the concentration range 0-0.003 g l^{-1}.

A linear sorption constant of 28 [cm^3 g^{-1}] or [g g^{-1} (clay] / g cm^{-3}] results in a reasonable fit in the depicted range (Figure 7.6), while a value of 29.14 produces a perfect fit for a concentration of 0.0005 g l^{-1}(Figure 7.7)

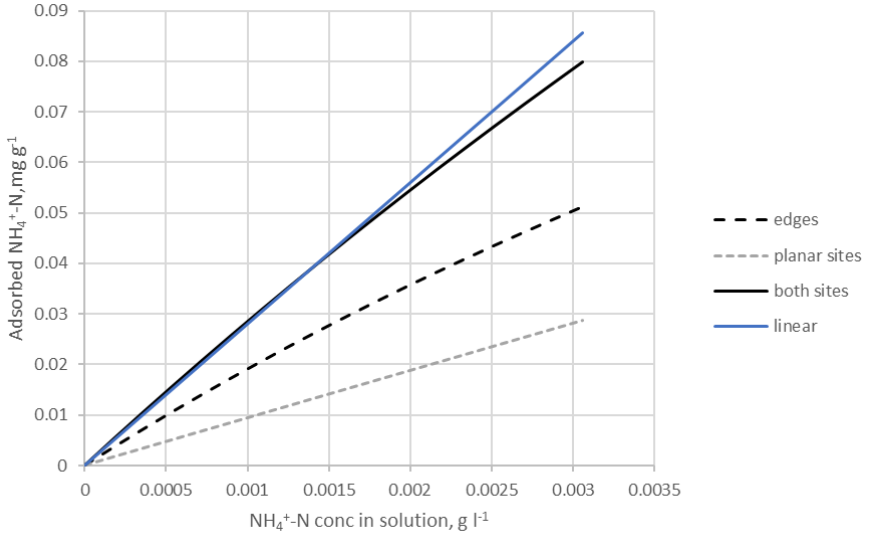

Figure 7.6. A linear sorption isotherm calculated with K_{clay} = 28 [cm^3 g^{-1}] compared to sorption calculated with the Schouwenburg and Schuffelen-model.

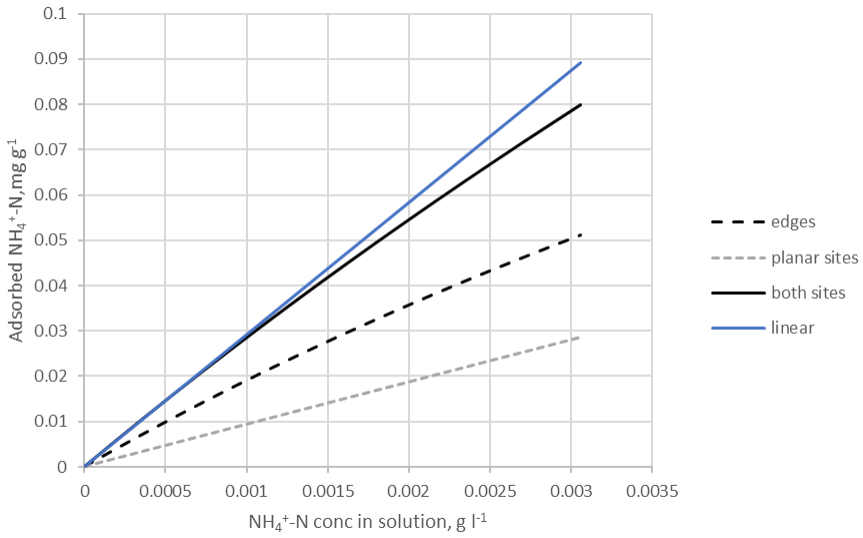

Figure 7.7. A linear sorption isotherm calculated with K_{clay} = 29.1417 [cm³ g⁻¹] compared to sorption calculated with the Schouwenburg and Schuffelen-model.

Based on the above, the default value for K_{clay} is 28 [cm^3 g^{-1}] in the default linear adsorption model for ammonium (*NH4*).

The default value for K_{OC} in the *NH4*-model builds on the following considerations:

- Cation exchange capacity and ammonium sorption are often linearly related (Young, 1964) (Al-Saedi et al., 2021). A rule of thumb is that CEC of clay is 0.5*clay % and 4*organic matter%, meaning that based on CEC, K_{OC}-should be 8 times as high. On the other hand, the affinity of ammonium to organic matter is smaller than to clay, which will reduce that number.
- The best quantitative study found (Young, 1964) concerns NH_3-gas-retention in 20 American soils, 76 horizons. When excluding the soils with andic features and 1:1-lattice clay, they find the following correlation between CEC and ammonia retention (also incl. 1:1-lattice clay)

  Surface soils (19): $NH_3\text{-}retention = 272.2 + 366.6 \cdot \%org.C + 48.17 \cdot \%clay$,

  For 69 horizons: $NH_3\text{-}retention = 388.8 + 226.1 \cdot \%org.C + 67.49 \cdot \%clay.$

  (R= 0.88 for surface soils and R=0.92 for all horizons):

- Assuming that the factors multiplied by organic C and clay, respectively, express the product of the effect of CEC and the sorption affinity, it can be inferred that for surface soils, K_{OC} should be about 7.6 times K_{clay}.
- As K_{OM} is equal to K_{OC}*0.587* (= 4.5), and CEC should be around 8, the affinity to organic matter would then be 50-60 % of that to clay in the topsoil. For all investigated soil horizons, the estimated K_{OC} is lower, 3.35 times K_{clay}. Here the affinity of organic matter seems to be lower, approximately 25 % of what it is to clay.

- This would indicate that the most reactive organic matter is present in the topsoil, and that a suggested value for K_{OC} in the topsoil could be 28*7.6=213 $cm^3\ g^{-1}$. For organic matter in the subsoil, the value is lower. The value for all horizons above produces a K_{OC} of 94, but for the subsoils alone, it could be lower than that. This is consistent with the fact that more reactive groups are removed over time as the level of decomposition increases. However, in most soils, the majority of the organic matter is present in the topsoil.

NB: The linear parameterization shown above with K_{clay}= 28 $cm^3\ g^{-1}$ and K_{OC} = 213 $cm^3\ g^{-1}$ are the default parameterization for ammonium sorption from version 7.0.7 (termed *NH4*). The earlier linear model parameterization (now termed *NH4_Hansen*) with K_{clay}= 117.116 $cm^3\ g^{-1}$ and K_{OC} = 117.116 $cm^3\ g^{-1}$ was erroneous. A test on the effect of the different parameterizations of the ammonium sorption on N dynamics are presented in appendix 7.1.

7.5 Nitrification

The microbial process whereby ammonium is oxidized into nitrate is referred to as nitrification. Ammonification, nitrification and denitrification, as well as possible interrelationships between the processes of nitrification and denitrification, are illustrated in Figure 7.8 based on results collected by Knowles (1978) and Nicholas (1978).

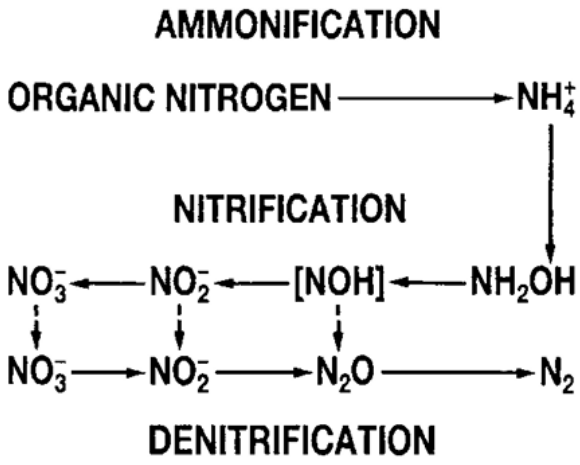

Figure 7.8. Ammonification, nitrification, denitrification, and possible interrelationships.

In well-aerated arable soils, with a relatively high water content (1.5<pF<2.5), pH in the range of 4-8, and soil temperature higher than 5°C, microbial activity is limited by the availability of organic carbon, and most ammonium is oxidized into nitrate as rapidly as it is formed by the process of ammonification. Thus, under such conditions, nitrite is rapidly oxidized into nitrate, and the release of N_2O during oxidation of ammonium is expected to occur mainly under conditions of reduced oxygen pressure. Assuming no oxygen stress, nitrification can be

considered as a single step process, which in Daisy is described using a Michaelis-Menten type of expression, with a nitrification rate (which depends on the temperature and pressure potential of the soil), a half-saturation constant, and the ammonium concentration:

$$\xi_n = \frac{V_n(T,h) \cdot N_{am}}{K_n + N_{am}} \tag{7.9}$$

where ξ_n [g N cm^{-3} h^{-1}] is the specific nitrification rate, $V_n(T,h)$ [g N cm^{-3} h^{-1}] is the maximum nitrification rate, K_n is a half-saturation constant (default: 5·10^{-5} [g N cm^{-3}], N_{am} is by default (option *soil*) the total ammonium concentration per volume [g N cm^{-3}] (sorbed and in solution), T is the soil temperature, and h is the pressure potential of the soil.

Daisy has a second option (*solute*), where nitrification is a function of the ammonium concentration in the soil water rather than the total ammonium concentration per volume. However, it does not have default values and thus requires parameterisation by the user.

Abiotic factors affecting nitrification in soils are substrate (NH_4^+, O_2, CO_2)-concentrations, pH, temperature and soil moisture content (Verstraete and Focht, 1977). In addition, naturally occurring inhibitory substances may affect nitrification. There is no evidence that pH in the range 5.5-8.0 and concentrations of CO_2 ever limit the nitrification process, whereas the concentration of O_2 clearly can be limiting. Thus, a temperature factor is specified, and a moisture-related factor is specified as a proxy for aeration conditions:

$$V_n(T,h) = V_n^* \cdot f_n^T(T) \cdot f_n^h(h) \tag{7.10}$$

V_n^* is the maximum nitrification rate at 10°C (default: 2.08*10^{-7} [g N cm^{-3} h^{-1}], calculated from 50 *10^{-7} [g N cm^{-3} d^{-1}]). The temperature and pressure potential functions were adopted from Flowers and O'Callaghan (1983), Tyler et al. (1959), Addiscott (1983), Miller and Johnson (1964), Sabey (1969) and Reichman et al. (1966).

Temperature function

The dependency on temperature resembles the temperature function for organic matter turnover from 6 to 37°C, but starts at 2°C rather than 0°C and declines above 37 degrees (Figure 7.9):

$$f_n^T = \begin{cases} 0 & T \leq 2 \\ 0.15 \cdot (T-2) & 2 < T \leq 6 \\ 0.1 \cdot T & 6 < T \leq 20 \\ exp(0.47 - 0.027 \cdot T + 0.00193 \cdot T^2) & 20 < T \leq 37 \\ f_n^T(37) \cdot \left(1 - \frac{(T-37)}{(60-37)}\right) & 37 < T \leq 60 \end{cases} \tag{7.11}$$

The modification of the function above 37°C is based on Van Veen and Frissel (1981). The user can specify a different temperature function, if required.

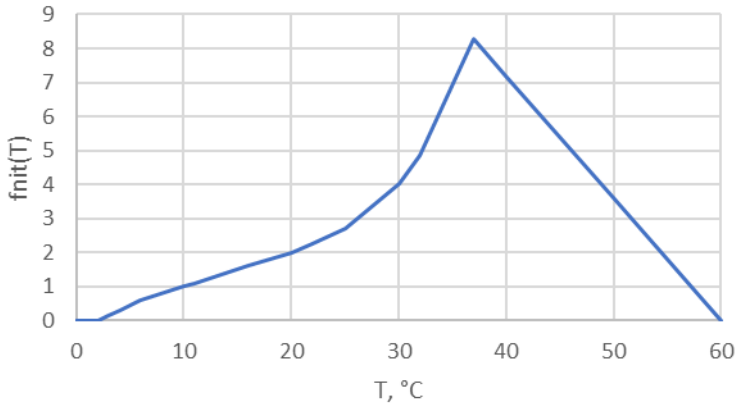

Figure 7.9: The dependency of nitrification on temperature.

Pressure potential function

The function related to the pressure potential (here expressed as a function of pF, where pF = $\log_{10}$(-h [cm])) increases from 0 to 1 in the interval pF= 0 to 1.5, stays at 1 until pF 2.5 and decreases linearly to 0 at pF 5, see eq. (7.12) and Figure 7.10. The user can specify a different water factor if required.

$$f_n^{pF} = \begin{cases} 0 & pF \leq 0 \\ pF/1.5 & 0 < pF \leq 1.5 \\ 1 & 1.5 < pF \leq 2.5 \\ 1 - (pF - 2.5)/2.5 & 2.5 < pF \leq 5.0 \\ 0 & 5.0 < pF \end{cases} \quad (7.12)$$

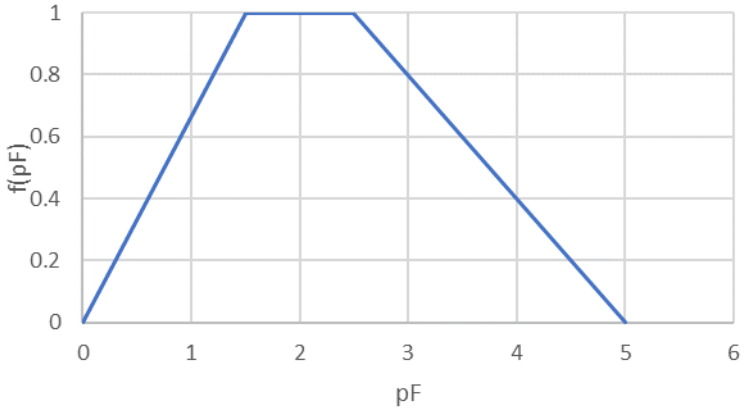

Figure 7.10: The dependency of nitrification on pF.

N_2O-formation via nitrification

The fraction of the nitrified amount that becomes N_2O is given as a constant (*N2O_fraction* []) with a default value of 0.02. This is within the range of other models (Xing et al., 2023). However, some recent, not published, comparisons with measurements indicate that the amount of generated N_2O may be similar to the total N_2O production from the soil with this parameterisation and thus overestimate the contribution from nitrification alone.

7.6 Denitrification

Biological denitrification is an important pathway by which nitrogen is lost from the soil to the atmosphere in the form of N_2 or related gasses, such as NO or N_2O, which are intermediate stages on the way from NO_3^- to N_2. Although the process has been studied extensively, the quantification of biological denitrification from fundamental microbial processes under field conditions is still far from perfect. However, it is well established (Fillery, 1983) that the rate of denitrification is related to the amount of easily decomposable organic matter, the volume of anaerobic microsites within an otherwise aerobic medium, the soil temperature, and the concentration of nitrate in the soil solution.

In the present model, denitrification is simulated by means of a rather simple index-type model considering the decomposition of organic matter, the volume of anaerobic microsites expressed simply in terms of soil water content, soil temperature, and the concentration of nitrate in soil solution. In accordance with Lind (1980), the potential denitrification rate of the soil (assuming anoxic conditions and ample nitrate concentration) is expressed as a linear function of the CO_2 evolution rate:

$$\xi_d^* = f_d^T(T) \cdot \alpha_d^* \cdot \xi_{CO_2} \tag{7.13}$$

where

ξ_d^* = the potential denitrification rate [g N cm^{-3}, h^{-1}],

α_d^* = a proportionality factor (default value 0.1 g Gas-N/g CO_2-C),

ξ_{CO_2} = the CO_2-evolution from the organic matter module [g CO_2-C cm^{-3}, h^{-1}],

$f_d^T(T)$ = a temperature function [], which by default is similar to the one for nitrification (eq. 7.11). It can be changed by the user.

This potential is then adjusted by a factor based on the amount of water present in the soil, which represents the gas exchange, $f_d^\theta(\theta)$, e.g. the soil water modifier function.

However, for denitrification to occur, nitrate must be present, and move by diffusion to the anaerobic sites, where denitrification takes place. The maximum transport occurs when the micro-sites act as zero sinks. The maximum transport of nitrate to micro-sites (ξ_t) [g N cm^{-3} h^{-1}] can therefore be assumed to be proportional to the nitrate concentration in the soil ($N_{NO_3\text{-}N} = \theta \cdot C_{NO_3\text{-}N}$, where $C_{NO_3\text{-}N}$ is the nitrate-N concentration in the soil solution). The increased tortuosity when the soil dries is of little consequence as denitrification is very limited in dry soil.

$$\xi_t = \left[\sum_i^n \theta A_i D \frac{C_{NO_3^- - N}}{\Delta r_i}\right] V^{-1} = K_d N_{NO_3^- - N} \tag{7.14}$$

where

θ = soil water content [cm^3 cm^{-3}]

D = diffusion coefficient [cm^2 h^{-1}]

A_i = surface area of microsites [cm^2]

$C_{NO3\text{--}N}$= conc. of NO_3^- -N in soil solution [g N cm^{-3}]

$N_{NO3\text{--}N}$ = conc. of NO_3^- -N in soil [g N cm^{-3}] = $\theta \cdot C_{NO3\text{--}N}$

Δr_i = diffusion distance to microsite i [cm]

n = number of microsites

V = soil volume [cm^3].

K_d = empirical proportionality factor [h^{-1}], default 0.020833 h^{-1}

The actual denitrification (ξ_d) [g N cm^{-3} h^{-1}] then becomes the minimum value of the adjusted potential and the availability of nitrate:

$$\xi_d = Min\left\{f_d^\theta(\theta) \cdot \xi_d^*; K_d \cdot N_{NO_3^- - N}\right\} \quad (7.15)$$

Soil water modifier function

The soil water modifier function has been changed over time in Daisy, and calibration is often required (Figure 7.11). The original parameterization (from 1990) only had a potential for denitrification when the relative water content in the soil was above 0.8. This water factor was adopted from Rolston et al. (1984).

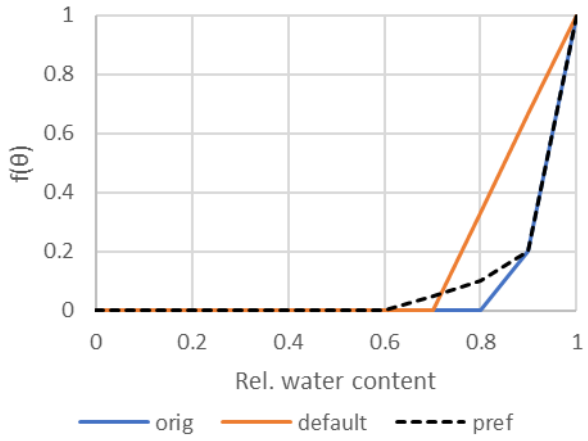

Figure 7.11: Examples of soil water modifier functions used in Daisy. "Orig" is the original parameterization from 1990, "default" is the present default and "pref" is a parameterization used in some recent projects.

In 2004, the soil water modifier function was calibrated based on measured data (Vinther and Hansen, 2004). This is the basis for the present default value (orange line in Figure 7.10). However, in recent years we have considered plough pans in many simulated soil profiles. This leads to higher water content in the A-horizon and very high denitrification rates, not consistent with typical measurements and observed plant growth. Hence, the parameterization represented by the broken line in Figure 7.10 has been found to produce more reasonable results across Danish soil types. Interestingly, it resembles the original parameterization, but the boundary for the required degree of saturation for denitrification to start is lower,

thus allowing some denitrification in sandy soils. Nevertheless, the soil water modifier factor is uncertain and should be considered a calibration factor.

Changing the water relationship for denitrification requires a chemistry definition as illustrated below:

```
(defchemistry low_denit multi
 (combine (N (reaction nitrification
                (denitrification
                 (water_factor (0.8 0.0) (0.9 0.2) (1.0 1.0))))))
)
```

"Slow" and "fast" CO_2-generation

In the default version of the standard denitrification model, all CO_2 generation is given the same weight in the calculation of the denitrification potential. However, it is possible in the same model to specify the anaerobic denitrification constant, α, separately for CO_2 coming from organic pools with fast turn-over and organic pools with slow turn-over, and to specify different fractions of nitrate converted (K) at each time step from fast and slow pools. Additionally, different soil water factors can be defined for the two types of pools. The parameter distinguishing between fast and slow pools is the "*CO2_threshold*" as specified in the "*organic*"-model. By default, this parameter is set at 0.0001 h^{-1}, equivalent to a half-life of 288.8 days. Consequently, the AOM pools and SMB2 typically belong to the fast pools, while the SOM pools and SMB1 belong to the slow pools (See Chapter 9).

Full denitrification below specified depth

Some soils contain material that leads to denitrification of (almost) all nitrate that passes through. The parameter "*redox_height*" [cm] allow specification of a depth (given as a negative number) below which nitrate will undergo immediate denitrification. This parameter is optional and is not implemented by default.

Parton1996

The ratio between N_2 and N_2O produced by the denitrification process is calculated as a function of NO_3^-concentration, $FR(NO_3)$, soil respiration, $FR(CO_2)$, and water-filled pose space $FR(WFPS)$, according to the model by Parton et al. (1996):

$$R_{N_2/N_2O} = \min(FR(\mathrm{N}_{\mathrm{NO}_3-\mathrm{N}}), FR(CO_{2-C})) * FR(WFPS) \quad (7.16)$$

The effect of NO_3^-concentration, $FR(\mathrm{N}_{\mathrm{NO}_3-\mathrm{N}})$, on the N_2/N_2O ratio is implemented as *P96NO3* following (Parton et al., 1996):

$$FR(\mathrm{N}_{\mathrm{NO}_3-\mathrm{N}}) = \left(1\left(0.5 + \frac{1\arctan\left(\pi 0.01(\mathrm{N}_{\mathrm{NO}_3-\mathrm{N}} - 190)\right)}{\pi}\right)\right)25 \quad (7.17)$$

where N_{NO_3-N} is the NO_3^-concentration in the soil [µg N g^{-1}].

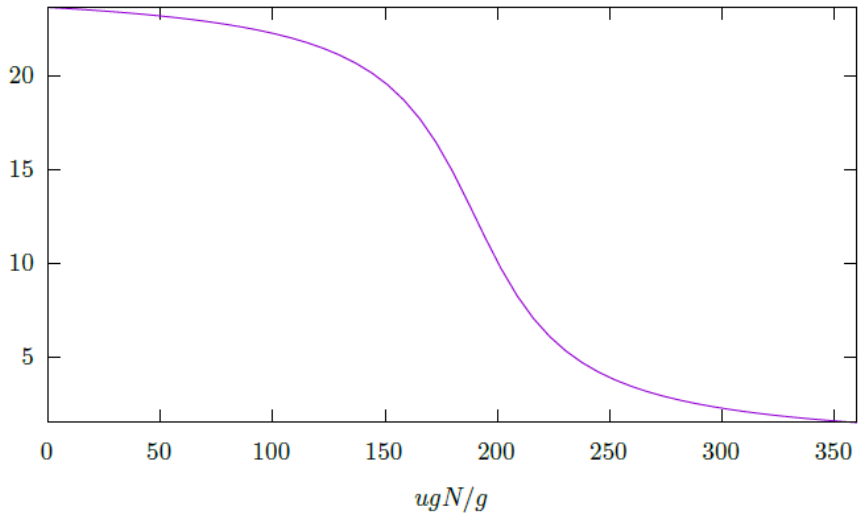

Figure 7.12: The NO_3 [µg N g^{-1}] effect on the N_2/N_2O-ratio.

The effect of soil respiration, $FR(CO_2)$, on the N_2/N_2O ratio is implemented as $P96CO2$ following (Parton et al., 1996):

$$FR(CO_{2-C}) = 13 + \frac{30.78 \arctan(\pi 0.07((CO_{2-C}) - 13))}{\pi} \quad (7.18)$$

where CO_{2-C} is the C lost through respiration [kg C ha^{-1} d^{-1}].

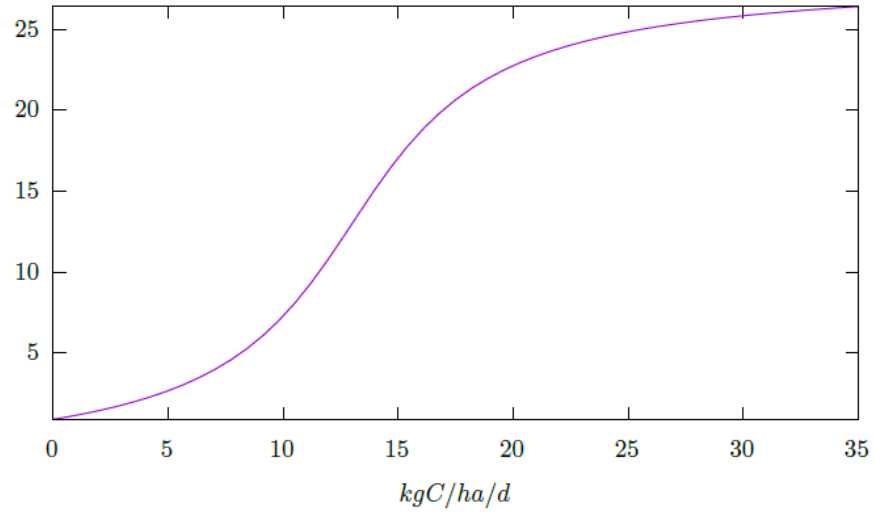

Figure 7.13: The CO_2 [kg C ha^{-1} d^{-1}] effect on the N_2/N_2O-ratio.

In Parton et al. (1996) the N_2O production is calculated for 30 cm tall columns, meaning area-based units such as [kg C ha^{-1} d^{-1}] for respiration (CO2_C) makes sense. In Daisy N_2O production is calculated for each position in the soil, with the unit for respiration [g C cm^{-3} h^{-1}]. To convert between the "per volume" units used by Daisy and the "per area" units used by Parton et al. (1996), the Daisy respiration are multiplied with a virtual column height, by default 30 cm (FR_CO2_depth). This conversion is done before the $FR(CO_{2-C})$ function is

called. The conversion from area-based functions to volume-based functions is perfectly safe as long as all involved functions are linear, which none of them are. So please use the Daisy estimation of N2O production with appropriate caution.

The effect of the water filled pore $FR(WFPS)$on the N_2/N_2O ratio is implemented as $P96WFPS$ following (Parton et al., 1996):

$$FR(WFPS) = \left(\frac{1.4}{13^{\left(13\left(\frac{17}{2.2WFPS}\right)\right)}} \right) \tag{7.17}$$

Where $WFPS$ is the water filled pore space [] given by θ/θ_{sat}.

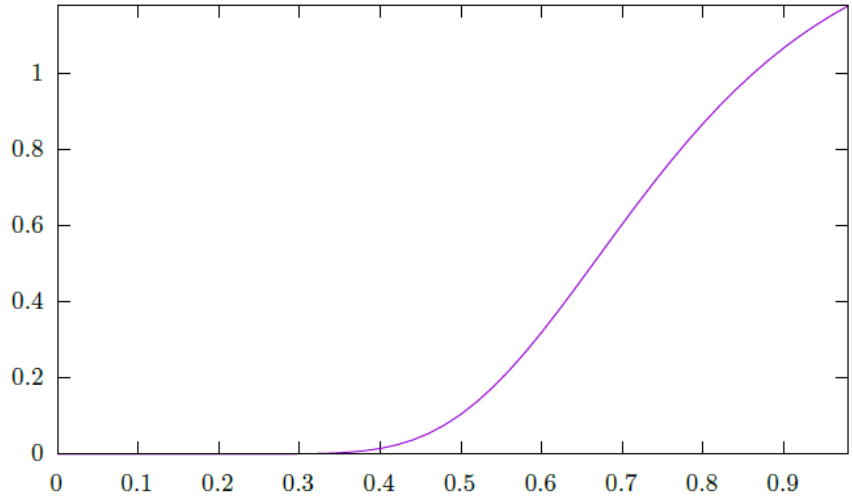

Figure 7.14: The water filled pore space (WFPS) [] effect on the N_2/N_2O-ratio

The final N_2O and N_2 gas fluxes from denitrification, ξ_{d-N_20} and ξ_{d-N_2} [g N cm^{-3} h^{-1}], are then calculated as follows (Parton et al., 1996):

$$\xi_{d-N_20} = \frac{\xi_d}{(1 + R_{N_2/N_2O})} \tag{7.20}$$

$$\xi_{d-N_2} = \frac{\xi_d}{\left(1 + \frac{1}{R_{N_2/N_2O}}\right)} \tag{7.21}$$

Where ξ_d is the actual denitrification (ξ_d) [g N cm^{-3} h^{-1}] given by eq. 7.15.

Parton1996 is the default model for calculating denitrification products (the *denprod* component of the denitrification model).

7.7 Nitrogen uptake by plants

The nitrogen uptake model can be considered as an analogy to the water uptake model. The upper limit for nitrogen uptake is the potential nitrogen uptake, which is assumed to be solely determined by the crop.

The actual nitrogen uptake may be equal to the potential nitrogen uptake, or it may be limited due to low availability of nitrogen in the soil (or, in some cases, by the root uptake rate).

Potential nitrogen uptake – demand

It is assumed that a plant will take up nitrogen until a certain nitrogen content in the plant is reached (Greenwood, 1986). The maximum nitrogen content is calculated as:

$$N_{pot} = \sum_{j=1}^{n} c_{j,pot} \cdot W_j \tag{7.22}$$

where

N_{pot} = upper limit of nitrogen content in the crop [kg N m^{-2}]
$c_{j,pot}$ = upper limit of nitrogen in plant part j [kg N kg^{-1} (DM)]
W_j = dry matter in plant part j [kg DM m^{-2}]
n = number of plant parts constituting the plant.

Values of $c_{j,pot}$ and W_j are obtained from the crop model ($c_{j,pot}$ is a parameter specified with a growth stage dependent plf-function, W_j is calculated in every timestep) (see Chapter 10). In the present context, a plant part can refer to the plant root system, leaves, stem, or storage organ of the plant.

It is assumed that the crop will take up nitrogen until the upper limit (N_{pot}) is reached if the nitrogen supply is ample and the root density is sufficient. Thus, the maximum uptake rate can be calculated from eq. (7.17).

$$\xi_u^* = Min\left\{\left(I^*_{NH_4^+-N} + I^*_{NO_3^-N}\right) \cdot \int_0^{dr} L \cdot dt;\ \frac{N_{pot}(t+\Delta t) - N_c(t)}{\Delta t}\right\} \tag{7.23}$$

where

ζ_u^* = maximum uptake rate of nitrogen [kg m^{-2} d^{-1}]
$I^*_{NH_4^+-N}$ = maximum uptake rate of NH_4^+-N per unit length of root [kg N m^{-1}(root) d^{-1}]
$I^*_{NO_3^-N}$ = maximum uptake rate of NO_3^--N per unit length of root [kg N m^{-1}(root) d^{-1}]
L = root length density [m m^{-3}]
dr = root depth [m]
N_c = actual nitrogen content in the crop [kg N m^{-2}]
t = time
Δt = time step [d^{-1}]

In eq. (7.17) it is assumed that $I^*_{NH_4^+\text{-}N}$ and $I^*_{NO_3^-\text{-}N}$ are constants, while the values of L and dr are obtained from the crop model. If the soil is able to supply nitrogen to the root surface at a rate equal to or greater than the maximum uptake rate, then the actual uptake rate equals the maximum uptake rate. Otherwise, the actual uptake rate is determined by the soil.

Nitrogen movement to root surfaces - supply

In the calculation of nitrogen movement from the bulk soil to the root surfaces, similar assumptions are made as those applied in the calculation of water movement from the bulk soil to the root surfaces. Thus, similar to root water uptake, it is assumed that only radial movement takes place, and this movement takes place only in the cylindrical soil volume surrounding the root. The radial transfer of nitrogen is approximated by a series of steady states. Assuming a steady state, we can formulate an advection-dispersion equation in cylindrical coordinates which takes the form of eq. (7.24):

$$\frac{1}{r}\cdot\frac{d}{dr}\left[rD_x^*\cdot\frac{dN_x}{dr}+rv_wC_x\right] \tag{7.24}$$

where

r = distance from center of root [m]

D_x^* = dispersion coefficient for substance x [$m^2\ s^{-1}$]

N_x =concentration of substance x in the soil [$kg\ m^{-3}$]

v_w = water flux density [$m\ s^{-1}$]

C_x = concentration of substance x in soil solution [$kg\ m^{-3}$]

When considering the uptake of nitrogen, the x in equation (7.24) can represent either NH_4^+-N or NO_3^--N. By introducing the buffer power with respect to substance x, as defined by eq. (7.25), into eq. (7.24), integration results in eq. (7.26).

$$b_x=\frac{dN_x}{dC_x} \tag{7.25}$$

$$I_x=2\pi r\cdot D_x\cdot\frac{dC_x}{dr}+q_w\cdot C_x \tag{7.26}$$

I_x = flux of substance x towards the root [$kg\ m^{-1}\ s^{-1}$],

b_x = buffer power of soil with respect to substance x, further described in eq. (7.34) and (7.35).

D_x = $D_x^*\cdot b_x$, b_x is in vol water per vol soil, i.e. [$m^3\ m^{-3}$], or []

q_w = $2\pi r\cdot v_w$, water flux towards the root [$m^3\ m^{-1}\ s^{-1}$]

The water flux towards the root is obtained from the soil water model (see chapter 4). Eq. (7.26) can be rearranged to give eq. (7.27). The solution to Eq. (7.27) is eq. (7.28).

$$\frac{dCx}{dr}=\frac{I_x}{2\pi D_x r}-\frac{q_wC_x}{2\pi D_x r} \tag{7.27}$$

$$C_x = \begin{cases} \frac{I_x}{2\pi D_x} ln(r) + B & \alpha = 0 \\ \frac{I_x}{q_w} + B \cdot r^{-\alpha} & \alpha \neq 0 \end{cases} \quad (7.28)$$

where B is an integration constant [kg m^{-3}] and $\alpha = q_w(2\pi D_x)^{-1}$ [].

The parameter α reflects the relationship between the effectiveness of mass transfer to diffusion. When α = 0, it indicates that mass-transfer has no contribution, and diffusion is the only mechanism responsible for transfer. Typically, α takes on a value between 0 and 0.1. The value $\alpha = 2$ has no special physical meaning but appears due to a mathematical singularity.

Assuming a concentration $C_x = C_{x,0}$ at the root surface at which $r = r_r$, the integration constant B is given by eq. 7.29. When this constant is introduced in eq. 7.28, it results in eq. 7.30.

$$B = \begin{cases} C_{x,0} - \frac{I_x}{2\pi D_x} ln(r_r) & \alpha = 0 \\ \left(C_{x,0} - \frac{I_x}{q_w}\right) r_r^{\alpha} & \alpha \neq 0 \end{cases} \quad (7.29)$$

$$C_x = \begin{cases} C_{x,0} + \frac{I_x}{2\pi D_x} ln\left[\frac{r}{r_r}\right] & \alpha = 0 \\ \frac{I_x}{q_w} + \left[C_{x,0} - \frac{I_x}{q_w}\right]\left[\frac{r}{r_r}\right]^{-\alpha} & \alpha \neq 0 \end{cases} \quad (7.30)$$

The average concentration in solution within the considered cylindrical soil volume is given by eq. (7.31):

$$\bar{C}_x = \frac{2\pi}{\pi(r_c^2 - r_r^2)} \int_{r_r}^{r_c} r \cdot C_x \cdot dr \quad (7.31)$$

$\bar{C}_x$ = average concentration in solution of substance x within a cylindrical soil volume [kg m^{-3}]

r_c = $(\pi \cdot L)^{-0.5}$, radius of considered cylindrical soil volume [m].

Assuming a constant value of α or if $\alpha = 0$ and that $I_x \cdot b_x \cdot (2 \cdot \pi \cdot D_x)^{-1}$ is independent of r, eq. (7.31) can be integrated, resulting in eq. (7.32).

$$\bar{C}_x = \begin{cases} C_{x,0} + \dfrac{I_x}{2\pi D_x}\left[\dfrac{\beta^2 ln(\beta)}{\beta^2-1} - \dfrac{1}{2}\right] & \alpha = 0 \\ \dfrac{I_x}{q_w} + \left[C_{x,0} - \dfrac{I_x}{q_w}\right] \cdot \dfrac{ln(\beta^2)}{\beta^2-1} & \alpha = 2 \\ \dfrac{I_x}{q_w} + \left[C_{x,0} - \dfrac{I_x}{q_w}\right] \cdot \dfrac{\beta^{2-\alpha}-1}{(\beta^2-1)\left(1-{}^{\alpha}/_{2}\right)} & \alpha \neq 0 \wedge \alpha \neq 2 \end{cases} \quad (7.32)$$

where

$$\beta = r_c \cdot r_r^{-1} = r_r^{-1}(\pi L)^{-1/2}$$

The β value characterizes the geometry of the system; high values of β correspond to sparce root systems, and low values of β correspond to high root density.

Actual nitrogen uptake, soil based

Eq. (7.32) can be rearranged to give eq. (7.33), from which the uptake rate of substance x per unit length of root is calculated, with the constraint that the uptake rate per unit root length cannot exceed the uptake capacity of the root.

$$I_x = \begin{cases} 2\pi D_x\left(\bar{C}_x - C_{x,0}\right) \cdot \left[\dfrac{\beta^2 ln(\beta)}{\beta^2-1} - \dfrac{1}{2}\right]^{-1} & \alpha = 0 \\ q_w \cdot \dfrac{(\beta^2-1)\cdot \bar{C}_x - C_{x,0}\cdot ln(\beta^2)}{(\beta^2-1) - ln(\beta^2)} & \alpha = 2 \\ q_w \cdot \dfrac{(\beta^2-1)\left(1-{}^{\alpha}/_{2}\right)\bar{C}_x - (\beta^{2-\alpha}-1)C_{x,0}}{(\beta^2-1)\left(1-{}^{\alpha}/_{2}\right) - (\beta^{2-\alpha}-1)} & \alpha \neq 0 \wedge \alpha \neq 2 \end{cases} \quad (7.33)$$

The uptake rate of substance x from a unit layer of soil can be calculated from eq. (7.34), after which the total uptake rate of substance x from the entire root zone is calculated from eq. (7.35).

$$\xi_{u,x} = Min(I_x^*, I_x) \cdot L \quad (7.34)$$

$$\zeta_{u,x} = \int_0^{d_r} \xi_{u,x} dz \quad (7.35)$$

where

ξ_{ux} = uptake rate of substance x per unit layer of soil [kg m^{-3} s^{-1}],

ζ_{ux} =uptake rate of substance x for the entire root zone [kg m^{-2} s^{-1}],

and dr, I_x^* and L are rooting depth [m], maximum root uptake rate of substance x [kg m^{-1} s^{-1}] and root density [m m^{-3}], respectively, as defined earlier.

Thus, the total nitrogen uptake rate from the entire root profile is:

$$\zeta_u = \zeta_{u,NH_4^+-N} + \zeta_{u,NO_3^--N} \quad (7.36)$$

where

ζ_u =total nitrogen uptake rate from the root zone [kg N m^{-2} s^{-1}]

$\zeta_{u,NH_4^+\text{-}N}$ = uptake rate of NH_4-N from the root zone [kg N m^{-2} s^{-1}]

$\zeta_{u,NO_3^-\text{-}N}$ = uptake rate of NO_3-N from the root zone [kg N m^{-2} s^{-1}]

Preferential uptake of ammonium

A basic assumption is that the uptake of NH_4^+-N has preference over the uptake of NO_3^--N. Consequently, uptake of NO_3^--N only takes place if $\zeta_{u,NH_4^+\text{-}N} < \zeta_u^*$. Thus, the potential uptake rate of NO_3^-N is given by eq. (7.37):

$$\zeta^*_{u,NO_3^-N} = \zeta^*_u - \zeta_{u,NH_4^+N} \tag{7.37}$$

where

$\zeta^*_{u,NO_3^-\text{-}N}$= potential uptake rate of NO_3-N from the root zone [kg N m^{-2} s^{-1}].

Mobility of nitrate and ammonium

In general, the concentration of NH_4^+-N in soil solution is lower than that of NO_3^--N. Furthermore, the mobility of NH_4^+-N in soil is low, and it is less mobile than NO_3^--N. Consequently, most of the nitrogen taken up by plants is in the form of NO_3^-N.

Solving the equation

In equation (7.33), two unknown variables appear, namely I_x and $C_{x,0}$. Thus, when using eq. (7.33), it is assumed that $C_{x,0}$ remains constant along the roots, while I_x may vary according to the variation in the other variables in the equation. Two situations may occur:

1. The nitrogen supply is ample and not limiting the uptake rate.
2. The nitrogen supply is limiting the uptake rate.

In the first situation, a common value of $C_{x,0}$ along the root is used to give the distribution of the uptake. The common value of $C_{x,0}$ is obtained by applying an iterative procedure ensuring that the total uptake is equal to the potential uptake of nitrogen.

In the second situation a common fixed value of $C_{x,0}$ is used. In this case, the calculation of I_x is straight forward. For both NH_4^+-N and NO_3^--N, the fixed value of $C_{x,0}$ is assumed to be zero, which means that the root acts as a zero-sink by default. However, this assumption can be modified, either by specifying a value for $C_{x,0}$ or by applying the “variable sink” option, as described later in this chapter.

In order to calculate the nitrogen uptake by plants, a number of crop, soil, and soil water parameters have to be known. The required crop parameters and variables are obtained from the crop model, while the soil water variables, including the soil water content and the soil water uptake by roots are obtained from the soil water model.

Dispersion coefficient

The required soil properties are the dispersion coefficient and the buffer power. In the calculation of solute transfer to the root surfaces, hydrodynamic dispersion is neglected. In this case, the dispersion coefficient is replaced by the diffusion coefficient, calculated as:

$$D_x = D_{x,e} \cdot \theta \cdot f_i \tag{7.37}$$

where

D_x = diffusion coefficient of substance x in soil [$m^2\ s^{-1}$]

$D_{x,e}$ = diffusion coefficient of substance x in free solution [$m^2\ s^{-1}$]

θ = volumetric soil water content [$m^3\ m^{-3}$]

f_i = tortuosity factor

The diffusion coefficient of nitrate in free solution is $2 \cdot 10^{-5}$ [$cm^2 s^{-1}$]. For ammonium, it is $1.8 \cdot 10^{-5}$ [$cm^2 s^{-1}$]).

Tortuosity factor

The tortuosity factor is assumed to be a soil characteristic depending on the soil water content:

$$f_i = \begin{cases} f_i^0 & \theta \le \theta_0 \\ f_i^0 + \alpha(\theta - \theta_0) & \theta > \theta_0 \end{cases} \tag{7.38}$$

In eq. (7.38) f_i^0, θ_0 and a are constants. A value of f_i^0 equal to 10^{-6} is selected arbitrarily, while α and θ_0 are parameters characterizing the soil.

Buffer power

In the case of NO_3^--N, it is assumed that no adsorption or desorption takes place. Hence, the buffer power with respect to NO_3^--N can be described as being equal to the volumetric soil water content.

$$b_{NO_3^- - N} = \frac{dN_{NO_3^- - N}}{dC_{NO_3^- - N}} = \frac{d\left(\theta \cdot C_{NO_3^- - N}\right)}{dC_{NO_3^- - N}} \tag{7.39}$$

For NH_4^+, the buffer capacity can be described as

$$b_{NH_4^+ - N} = \frac{dN_{NH_4^+ - N}}{dC_{NH_4^+ - N}} = \frac{x_c \rho \cdot V_p \cdot K_p}{\left(K_p + C_{NH_4^+ - N}\right)^2} + \frac{x_c \rho \cdot V_e \cdot K_e}{\left(K_e + C_{NH_4^+ - N}\right)^2} + \theta \tag{7.40}$$

where

$N_{NH_4^+}$-N = concentration of NH_4^+-N in soil [kg N m^{-3} (soil)]

x_c = clay content in soil

ρ = soil dry bulk density [kg m^{-3}]

In calculations of diffusion coefficient and buffer power, bulk values of the soil water content are used. Furthermore, the average values of the concentration of NH_4^+-N and NO_3^--N, respectively, are assumed to be equal to the bulk values of the corresponding concentrations used in the solution of the convection-dispersion equation.

$C_{x,0}$ at the root surface in eq. (7.29) is by default set to 0 but may be given a value using the parameters *NO3_root_min* and *NH4_root_min* [g N cm^{-3}]. Furthermore,

a minimum concentration near roots can be defined for luxury uptake in the reproductive phase (*NO3_root_min_luxury* and *NH4_root_min_luxury* [g N cm^{-3}]). By default the last two parameters are identical to the first two parameters.

The variable sink option

The variable sink option builds on an article by Tsay et al. (2007), describing the transport of nitrate across the root boundary for *Arabidopsis*. The uptake kinetics of nitrate is governed by a dual-affinity system viz. a high affinity system with a low uptake capacity and a low affinity system with high uptake capacity. The system can be described by Michaelis-Menten kinetics, as shown in eq. (7.41):

$$I_{NO_3^- - N} = \frac{F_1 C_{NO_3^- - N,0}}{K_1 + C_{NO_3^- - N,0}} + \frac{F_2 C_{NO_3^- - N,0}}{K_2 + C_{NO_3^- - N,0}} \tag{7.41}$$

where *F* and *K* refer to the max uptake rate and the half-saturation constant, respectively, and the subscripts 1 and 2 refer to the high affinity system and low affinity system, respectively. I_{NO_3} is the uptake rate for nitrate and $C_{NO_3,0}$ is the concentration of nitrate at the root surface.

Eq. (7.33) can be written as a linear relation between root uptake, I_x, and $C_{x,0}$, i.e:

$$I_x = a_z + b_z \cdot C_{x,0} \tag{7.42}$$

where

$$a_z = \begin{cases} 2\pi D \left[\dfrac{\beta^2 ln(\beta)}{\beta^2 - 1} - \dfrac{1}{2}\right]^{-1} \bar{C}_x & \alpha = 0 \\ 4\pi D \dfrac{(\beta^2 - 1)}{(\beta^2 - 1) - ln(\beta^2)} \bar{C}_x & \alpha = 2 \\ 2\pi D \dfrac{\alpha(\beta^2 - 1)\left(1 - {}^{\alpha}/_{2}\right)}{(\beta^2 - 1)\left(1 - {}^{\alpha}/_{2}\right) - (\beta^{2-\alpha} - 1)} \bar{C}_x & \alpha \neq 0 \wedge 2 \end{cases} \tag{7.43}$$

and

$$b_z = \begin{cases} -2\pi D \left[\dfrac{\beta^2 ln(\beta)}{\beta^2 - 1} - \dfrac{1}{2}\right]^{-1} & \alpha = 0 \\ -4\pi D \dfrac{ln(\beta^2)}{(\beta^2 - 1) - ln(\beta^2)} & \alpha = 2 \\ -2\pi D \dfrac{\alpha(\beta^{2-\alpha} - 1)}{(\beta^2 - 1)\left(1 - {}^{\alpha}/_{2}\right) - (\beta^{2-\alpha} - 1)} & \alpha \neq 0 \wedge 2 \end{cases} \tag{7.44}$$

Equating 7.41 and 7.42 yields

$$a_z + b_z C_{x,0} = \frac{F_1 C_{x,0}}{K_1 + C_{x,0}} + \frac{F_2 C_{x,0}}{K_2 + C_{x,0}} \tag{7.45}$$

assuming, in this case that x is nitrate. Characterizing nitrate uptake Tsay et al. (2007) suggests values of 50 µM (0.7 mg NO^-_3-N/L) and 5000 µM(70 mg NO^-_3-N/L) for the half-saturation constant for the high and for the low affinity system, respectively. The maximum uptake rates are more uncertain. Based on preliminary calibrations, we suggest that F1 makes up about 10 % of the maximum uptake rate specified. Equation (7.45) can be solved for $C_{x,0}$, and subsequently, I_x can be calculated using eq. (7.41) or eq. (7.42).

The equations for the variable sink-system stem only from studies of nitrate. To avoid using the variable sink option for both nitrate and ammonium, the model should be specified for nitrate while the fixed sink model should be specified for ammonium.

"none"

Solute uptake can be disabled by using the *none* option.

Multiple crops

In case more than one crop is present, each crop takes up nitrogen independent of the other. Total uptake is thus the sum of the uptake of each crop (superposition). This method is chosen because plant uptake is a "forward" or "explicit" solution. The uptake is calculated based on the condition in the beginning of the time interval and is considered constant during the interval. The condition in the beginning of the time interval is independent of what happens during the time interval.

7.8 Parameter overview

Table 7.1. Related Parameter names in Daisy.

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
Canopy dissipation rate	General parameter for the subgroup "nutrient" under "chemical"	Chemical_std_C	*canopy_dissipation_rate*	0	[h^{-1}]
Canopy washoff coefficient	General parameter for the subgroup "nutrient" under "chemical"	Chemical_std_C	*canopy_washoff_coefficient*	1	[]
Decomposition rate	General parameter for the subgroup "nutrient" under "chemical"	Chemical_std_C	*decompose_rate*	0	[h^{-1}]
Diffusion coefficient	Specified separately for ammonium and nitrate	chemical_std_C	*diffusion_coefficient*	NH_4^+: 1.8E-05 NO_3^-: 2.0E-05	[$cm^2\ s^{-1}$]
Initial concentrations	Initial concentration of NH_4^+-N and NO_3^--N in soil water	chemical_std_C	*initial_NH4* *initial_NO3*	0.5E-06 5.0E-06	[g NH4-N cm^{-3}] [g NO_3-N cm^{-3}]
mineral	A sub-model for mineral fertilizers	am.C	*weight* *NH4-fraction* *volatilization*	0 User specified (lib) 0	[kg N ha^{-1}] [] []
J^C_{drydep}	Dry deposition (general)	weather	*NH4DryDep* *NO3DryDep* *Deposition* *DepDry* *DepDryNH4*	Optional input Optional input total deposition with fractions for dry deposition of total and amm. fraction of this.	[kg N $ha^{-1}y^{-1}$] [kg N $ha^{-1}y^{-1}$] [kg N ha^{-1}] [] []

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
c_{wetdep}	Wet deposition, conc. of solute in precipitation	weather	*NH4WetDep* *NO3WetDep*	Optional input Optional input	[ppm = mg $mm^{-1}m^{-2}$]
Adsorption model for NH_4	Choice of all implemented models allowed	chemical_std_C	*adsorption*	NH4	
x_c	Clay content, eq. 7.7.	adsorption_vS_S	*clay*	Defined for horizon	[fraction]
ρ_b	Bulk density, eq. 7.7.	adsorption_vS_S	*Dry_bulk_density*	Defined for horizon	[g cm^3]
V_p	Absorption capacity of planer sites on clay, eq. 7.7.	adsorption_vS_S	-	$6 \cdot 10^{-3}$	[g (g clay)$^{-1}$]
V_e	Absorption capacity of edges of clay, eq. 7.7.	adsorption_vS_S	-	$1.8 \cdot 10^{-3}$	[g (g clay)$^{-1}$]
K_p	Half saturation constant, planer sites, eq. 7.7.	adsorption_vS_S	-	63	[g m^{-3}]
K_e	Half saturation constant, edges, eq. 7.7.	adsorption_vS_S	-	14	[g m^{-3}]
K_{clay}	Linear sorption constant for clay, given per gram clay	adsorption NH4	*K_clay*	28	[g g^{-1} (clay] / g cm^{-3}]
K_{OC}	Linear sorption constant for organic carbon, given per gram organic carbon.	adsorption NH4	*K_OC*	213	[g g^{-1} (OC] / g cm^{-3}]
K_n	Half saturation constant, nitrification, eq. (7.9)	nitrification_soil.C	*k*	$5 \cdot 10^{-5}$	[g N cm^{-3}]
V_n^*	Maximum nitrification rate at 10°C, eq. (7.10).	nitrification_soil.C	*K_10*	$2.08333 \cdot 10^{-7}$	[g N cm^{-3} h^{-1}]
f_n^T	Temperature factor for nitrification – eq, (7.10) only specified if default is not used.	nitrification_soil.C	*(heat_factor)*	Default values, see eq. (7.11)	plf [dg C -> [fraction]]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
f_n^{pF}	Pressure potential function – eq. (7.10) only specified if default is not used.	nitrification_soil.C	*(water_factor)*	Default values, see eq. (7.12),	plf [cm -> [fraction]]
N_2O-fraction	Fraction of nitrified N ending up as N_2O	nitrification_soil.C	*N2O_fraction*	0.02	[]
α_d^*	Anaerobic denitrification constant for slow pools, default for all pools if alpha_fast is not defined. Eq.7.13.	reaction_denit.C	*alpha*	0.1	[g Gas-N/g CO_2-C]
	Anaerobic denitrification constant for fast pools	reaction_denit.C	*alpha_fast*	0.1, optional parameter	[g Gas-N/g CO_2-C]
K_d	Maximum fraction of nitrate converted at each time step from slow pools, eq. 7.14	reaction_denit.C	*K*	0.00833	[h^{-1}]
	Maximum fraction of nitrate converted at each time step from fast pools	reaction_denit.C	*K_fast*	0.00833, optional parameter	[h^{-1}]
f_d^T	Temperature factor for denitrification – only specified if default is not used.	reaction_denit.C	*(heat_factor)*	Identical to f_n^T, see eq. (7.11)	
$f_d^\theta(\theta)$	Dependency of denitrification on relative water content in soil, fig. 7.10.	reaction_denit.C	*(water_factor)*	((0.7 0) (1 1))	plf (relative water content[] ->fraction[]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
	Dependency of denitrification on relative water content in soil for fast pools	reaction_denit.C	*(water_factor_fast)*	Optional parameter. By default, identical to *water_factor*	plf (relative water content[] ->fraction[]
	Height (negative number) below which redox processes start. All nitrate is removed immediately.	reaction_denit.C	*Redox_height*	By default, this function is not used	[cm]
	Depth used for converting CO2 from value to area units.	Parton1996	*FR_CO2_depth*	30	[cm]
	Threshold value for turn-over rates of organic pools, above which the pools are considered "fast".	Organic_std.C	*CO2_threshold*	0.0001	[h^{-1}]
$I^*_{NH_4^+\text{-}N}$	Maximum NH_4^+ uptake per unit root length	RootSystem	*MxNH4Up*	$2.5\ 10^{-7}$	[g cm^{-1} h^{-1}]
$I^*_{NO_3^-\text{-}N}$	Maximum NO_3^- uptake per unit root length	RootSystem	*MxNO3Up*	$2.5\ 10^{-7}$	[g cm^{-1} h^{-1}]
	Choice of root uptake model for NH4-uptake	RootSystem, solute uptake component	*NH4_uptake*	By default, identical to the NO3-uptake model.	
	Choice of root uptake model for NO3-uptake	RootSystem, solute uptake component	*NO3_uptake*	By default, the "fixed_sink" description is selected	
Fixed sink	A model that finds the highest value of CRoot that meets the	solute_uptake	*fixed_sink*	Min value set in CrpN	[g N cm^{-3}]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
	N-demand, assuming a specified minimum concentration along the root.				
$C_{x,0}$, $x = NO_3^-$	Minimum NO_3^- concentration along the root	CrpN	*NO3_root_min*	0	g N cm^{-3}
$C_{x,0}$, $x = NH_4^+$	Minimum NH_4^+ concentration along the root	CrpN	*NH4_root_min*	0	g N cm^{-3}
	Minimum NO_3^- concentration along the root for luxury uptake in reproductive phase	CrpN	*NO3_root_min_luxury*	*NO3_root_min*	g N cm^{-3}
	Minimum NH_4^+ concentration along the root for luxury uptake in reproductive phase	CrpN	*NH4_root_min_luxury*	*NH4_root_min*	g N cm^{-3}
Variable-sink	Dual affinity transport across root boundary	Solute-uptake	*variable_sink*		
K_1	K parameter for high affinity uptake, eq. (7.36)	variable_sink	*K1*	$7\ 10^{-7}$	[g N cm^{-3}]
K_2	K parameter for low affinity uptake, eq. (7.36)	variable_sink	*K2*	$7\ 10^{-5}$	[g N cm^{-3}]
F1 and F2	Max uptake rates for the two systems across the root, in Daisy specified as fraction of max uptake allocated to high affinity process.	variable_sink	*F_relative*	0.1	[]

Original text from	A10 and “Daisy Description”	
Updated by	date	For Daisy version
Styczen, M & Holbak, M.	2025 06 04	7
Holbak, M.	2026 03 20	7

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