Addendum to Alterra Report 983
"Prediction of Nitrogen and Phosphorus leaching to groundwater and surface waters; Process descriptions of the animo4.0 model. by P. Groenendijk, L.V. Renaud and J. Roelsma, 2005"

Page 44-47 is replaced by the following text:

The amount of nitrogen present in the shoot system can be found from the remaining quantity after the last cutting and the nitrogen quantity extracted from the soil partitioned to the shoots. The biomass present in the grass shoot system is simulated by the simple grassland production module.

Nitrate uptake

The concept of supply potential is based on the assumption that total uptake is equivalent to the sum of convective transport and diffusive transport to plant roots.

$$R_{u,NO3} = R_{u,c} + R_{u,d} \tag{5.20}$$

where the subscripts c and d denote resp. the convective and diffusive transport. The convective uptake transport of nitrate in soil compartment i is described as Fickian transport:

$$R_{u,c} = \sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i} \tag{5.21}$$

where:

$q_{ep,i}$	:	plant evaporation flux of compartment i	(m d^{-1})
Δz_i	:	thickness of compartment i	(m)
$\bar{c}_{NO3,i}$	:	time averaged nitrate concentration in compartment i	(kg m^{-3})
$\sigma_{NO3,i}$	:	*transpiration concentration stream factor* corresponding to convective nitrate uptake	(-)

When the soil nitrate concentration exceeds the nitrate concentration of root liquids, the diffusive nitrate uptake is governed by:

$$R_{u,d} = \theta_i \; k_{gr,dif} \bar{c}_{NO3,i} - \min\left(\sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i}, \theta_i \; k^*_{gr,dif} \; c_{pl} \right) \tag{5.22}$$

where the "forward" diffusion rate is proportional to a first order rate constant $k_{gr,dif}$ (d^{-1}) and the "backward" diffusion rate is proportional to a constant $k^*_{gr,dif}$ (d^{-1}) which can be chosen smaller than $k_{gr,dif}$. Precaution is taken to avoid a "backward" diffusion rate from the plants roots to the bulk soil that exceeds the convective transport rate. The internal concentration in plant roots has been assumed proportional to the concentration in plant shoots and the ratio between the nitrogen fractions in plant roots and plant shoots.

In numerical computation schemes, the soil system is schematized to homogeneous compartments with thickness Δz_i. The nitrate uptake in compartment *i* is then determined by:

$$R_{u,c} = \sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i} + \theta_i \ k_{gr,dif} \bar{c}_{NO3,i} - \min\left(\sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i}, \theta_i \ k^*_{gr,dif} \ c_{pl} \right) \qquad (5.23)$$

The uptake process has been incorporated in the conservation and transport equation by defining the overall *transpiration concentration stream factors* $\sigma^*_{NO3,i}$ per soil compartment *i* and a zero-order production term to be added to $k_{0,NO3,i}$. When the nitrogen accumulation has not lead to nitrogen contents above a defined threshold level, the uptake parameters in the transport and conservation equation are defined by:

$$\sigma^*_{NO3,i} = \sigma_{NO3,i} + \theta_i \ k_{gr,dif} \frac{\Delta z_i}{q_{ep,i}} \qquad (5.24a)$$

$$k^*_{0,NO3,i} = k_{0,NO3,i} + \min\left(\sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i}, \theta_i \ k^*_{gr,dif} \ c_{pl} \right) \qquad (5.24b)$$

The internal concentration in grass shoots c_{pl} (kg m^{-3}) is calculated from a relation between the concentration and the N-fraction in the shoots, based on experimental data. The internal plant concentration is assumed to be proportional to the nitrate fraction of the shoots ($f_{pl,NO3}$):

$$c_{pl} = \frac{f_{ds}}{1 - f_{ds}} 1000 \, f_{pl,NO3} \qquad (5.25)$$

where f_{ds} is the dry matter content of the biomass. The nitrate fraction in the shoots is related to the total nitrogen fraction. In an analysis of experimental field data of Ruurlo (Fonck, 1982b,a), both the NO_3-N concentrations (kg m^{-3}) and the total nitrogen fractions have been calculated as a annual average values, based on 7 cuttings per field plot (5.2).

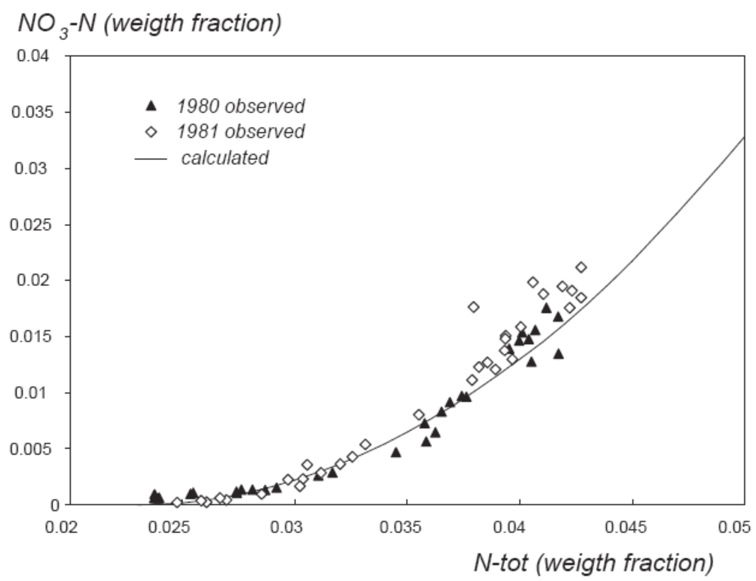

Figure 5.2: *Nitrate-N weight fraction (f_{pl,NO_3}) as a function of total nitrogen weight fraction ($f_{pl,N_{tot}}$) in grass shoots*

The nitrate weight fraction $f_{pl,NO3}$ is related to the total nitrogen fraction $f_{pl,Ntot}$ according to a fitted relation:

$$
\begin{aligned}
f_{pl,N_{tot}} \le 0.023 \quad & f_{pl,NO_3} = \quad 0 \\
0.023 < f_{pl,N_{tot}} \le 0.04 \quad & f_{pl,NO_3} = \quad 45(f_{pl,N_{tot}} - 0.023)^2 \\
f_{pl,N_{tot}} > 0.04 \quad & f_{pl,NO_3} = \quad \frac{0.06561}{1 \ + \ e^{-140 f_{pl,N_{tot}} + 7}}
\end{aligned}
\qquad (5.26)
$$

Ammonium uptake

The ammonium uptake is based on convective transport (*concentration* × *water flow*), diffusive transport and takes account for the quantity adsorbed to soil particles. The internal ammonium plant concentration is assumed zero. The uptake per soil compartment for a certain time step:

$$R_{u,NH4} = \sigma_{NH4} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NH4,i} + \left(\theta_i + \rho_{d,i} K_{e,NH4,i}\right) k_{gr,dif} \bar{c}_{NH4,i} \qquad (5.27)$$

where:

$K_{e,NH4,i}$	:	linear NH_4 adsorption coefficient in compartment *i*	(m^3 kg^{-1})
$\bar{c}_{NH4,i}$	:	time averaged NH_4 concentration in compartment *i*	(kg m^{-3})
σ_{NH4}	:	*transpiration concentration stream factor* corresponding to convective ammonium uptake	(-)

The uptake process has been incorporated in the conservation and transport equation by defining the overall *transpiration concentration stream factors* $\sigma^*_{NH4,i}$ per soil compartment *i*. When the nitrogen accumulation has not lead to nitrogen contents above a defined threshold level, the uptake parameters are defined by:

$$\sigma^*_{NH4,i} = \sigma_{NH4,i} + k_{gr,dif} \frac{\Delta z_i}{q_{ep,i}} \left(\theta_i + \rho_{d,i} K_{e,NH4,i}\right) \qquad (5.28)$$

When the soil mineral nitrogen availability exceeds the crop requirement, the uptake parameter σ_{NH_4} will be adjusted on the basis of a defined maximum requirement. Due to electro-neutrality considerations, a preference for nitrate uptake is assumed. Nitrate and ammonium soil availabilities (Φ_{NO_3} and Φ_{NH_4}) are defined according to Eq. 5.7. Maximum uptake requirement Ω_N^{max} and the mean uptake requirement Ω_N^{mean} variables are introduced:

$$\Omega_N^{max} = Q_s(t) f_{N,s}^{max} + Q_r(t) f_{N,r}^{max} - U(t_0) \quad (5.30)$$

$$\Omega_N^{mean} = Q_s(t) \frac{f_{N,s}^{max} + f_{N,s}^{min}}{2} + Q_r(t) \frac{f_{N,r}^{max} + f_{N,r}^{min}}{2} - U(t_0) \quad (5.31)$$

Based on these defined uptake requirements and the availability of nitrogen, the ammonium uptake factor is determined. If the nitrate availability exceeds the maximum requirement, no ammonium will be taken up:

$$\Phi_{NO_3} > \Omega_N^{max} \Rightarrow \sigma_{NH_4} = 0 \quad (5.32)$$

If the nitrate availability is less than the maximum nitrogen requirement, but the sum of nitrate and ammonium availability is greater than the maximum requirement, the uptake parameter is calculated by:

$$\Phi_{NO_3} < \Omega_N^{max} < \Phi_{NO_3} + \Phi_{NH_4} \Rightarrow \sigma_{NH_4} = \frac{\Omega_N^{max} - \Phi_{NO_3}}{\Phi_{NH_4}} \quad (5.33)$$

When the sum of nitrate and ammonium availability is less than the maximum nitrogen requirement, but greater than the mean nitrogen requirement:

$$\Omega_N^{mean} < \Phi_{NO_3} + \Phi_{NH_4} < \Omega_N^{max} \Rightarrow \sigma_{NH_4} = 1 \quad (5.34)$$

In all other situations the *transpiration concentration stream factor* for ammonium σ_{NH_4} takes the maximum value ($\sigma_{NH_4}^{max}$).

Phosphorus uptake

Uptake of mineral phosphate by plant roots has been described closely related to the nitrogen uptake. However, for phosphorus no accumulation that can become available for future growth has been assumed.

$$R_{u,P} = \sigma_P \frac{q_{ep}}{\Delta z} c_{PO4} \quad (5.35)$$

The uptake factor σ_P is defined on the basis of soil availability and crop requirement. Soil availability of phosphate is calculated as the sum of the amounts present in the liquid phase, the fast sorption pool $X_P^{eq.s}$ (equilibrium) and the precipitation pool X_P^{prec}. The phosphorus uptake under unconstrained conditions equals the mineral P availability:

$$U(t_0 + \Delta t) = U(t_0) + \Phi_{PO4} \quad (5.36)$$

where the mineral phosphorus availability is approximated by:

$$\Phi_{PO4} = \sum_{i=1}^{Nr} \left(1 + \frac{\rho_{d,i} \, K_{e,i}^{app}}{\theta_i} \right) q_{ep,i} \bar{c}_{PO4,i} \Delta t \quad (5.37)$$

with K_e^{app} as the apparent linear sorption coefficient defined by Eq. 5.13. The phosphate requirement for plant growth is defined as the gross dry matter production multiplied by the actual phosphorus content of shoots and roots. The P-fractions relate to the total N-fractions according to:

$$
\begin{aligned}
f_{P,s} &= \frac{f_{P,s}^{min} + f_{P,s}^{max}}{f_{N,s}^{min} + f_{N,s}^{max}} \left(f_{pl,N_{tot}} - f_{pl,NO_3}\right) \\
f_{P,r} &= \frac{f_{P,r}^{min} + f_{P,r}^{max}}{f_{N,r}^{min} + f_{N,r}^{max}} \frac{f_{N,r}^{min}}{f_{N,s}^{min}} \left(f_{pl,N_{tot}} - f_{pl,NO_3}\right) \qquad (5.38)
\end{aligned}
$$

Based on the demand and the availability, the plant uptake parameter σ_P is defined by:

$$
\begin{aligned}
\Phi_P > \Omega_P \quad &\Rightarrow \quad \sigma_P = \frac{\Omega_P}{\Phi_P} \\
\Omega_P > \sigma_P^{max}\Phi_P \quad &\Rightarrow \quad \sigma_P \; = \; \sigma_{P,max} \qquad (5.39)
\end{aligned}
$$

The maximum value of the plant parameter (σ_P^{max}) has been set to one in a number of regional model applications.

5.2.3 Nutrient limitation of biomass production

The nitrogen uptake under unconstrained conditions equals to the mineral nitrogen availability:

$$
\begin{aligned}
U(t0+\Delta t) = U(t) &+ \sum_{i=1}^{Nr} \sigma^*_{NH4,i} q_{ep,i} \bar{c}_{NH4,i} \Delta t + \sum_{i=1}^{Nr} \sigma^*_{NO3,i} q_{ep,i} \bar{c}_{NO3,i} \Delta t \\
&+ \min\left(\sigma_{NO3,i} \frac{q_{ep,i}}{\Delta z_i} \bar{c}_{NO3,i}, \theta_i \; k^*_{gr,dif} \; c_{pl} \right) \Delta z_i \Delta t \qquad (5.40)
\end{aligned}
$$

with K_e^{app} as the apparent linear sorption coefficient defined by Eq. 5.13. The phosphate requirement for plant growth is defined as the gross dry matter production multiplied by the actual phosphorus content of shoots and roots. The P-fractions relate to the total N-fractions according to:

$$
\begin{aligned}
f_{P,s} &= \frac{f_{P,s}^{min} + f_{P,s}^{max}}{f_{N,s}^{min} + f_{N,s}^{max}} \left(f_{pl,N_{tot}} - f_{pl,NO_3}\right) \\
f_{P,r} &= \frac{f_{P,r}^{min} + f_{P,r}^{max}}{f_{N,r}^{min} + f_{N,r}^{max}} \frac{f_{N,r}^{min}}{f_{N,s}^{min}} \left(f_{pl,N_{tot}} - f_{pl,NO_3}\right) \qquad (5.38)
\end{aligned}
$$

Based on the demand and the availability, the plant uptake parameter σ_P is defined by:

$$
\begin{aligned}
\Phi_P > \Omega_P \quad &\Rightarrow \quad \sigma_P = \frac{\Omega_P}{\Phi_P} \\
\Omega_P > \sigma_P^{max}\Phi_P \quad &\Rightarrow \quad \sigma_P \; = \; \sigma_{P,max} \qquad (5.39)
\end{aligned}
$$

The maximum value of the plant parameter (σ_P^{max}) has been set to one in a number of regional model applications.

The nitrogen requirement for plant growth is defined as the gross dry matter production multiplied by the actual nitrogen content of shoots and roots, resp $f_{N,s}$ and $f_{N,r}$:

$$\Omega_N = f_{N,s} \int_{t_0}^{t_0+\Delta t} \left(\frac{dQ_s(t)}{dt} + W \right) dt + f_{N,r} \int_{t0}^{t0+\Delta t} \left(\frac{dQ_r(t)}{dt} + k_{gr,decease} \right) dt \qquad (5.41)$$