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SURFATM-NH₃: a model combining the surface energy balance and bi-directional exchanges of ammonia applied at the field scale

**E. Personne¹, B. Loubet¹, B. Herrmann², M. Mattsson³, J. K. Schjoerring³,
E. Nemitz⁴, M. A. Sutton⁴, and P. Cellier¹**

¹UMR Environment et Grandes Cultures/INRA – AgroParisTech, 78 850 Thiverval Grignon, France

²Agroscope Reckenholz-Tänikon Research Station ART, Reckenholzstrasse 191, 8046 Zürich, Switzerland

³Plant and Soil Science Laboratory, University of Copenhagen, Faculty of Life Sciences, Thorvaldsensvej 40, 1871 Frederiksberg C, Copenhagen, Denmark

⁴Centre for Ecology and Hydrology, Edinburgh Research Station, Bush Estate, Penicuik, Midlothian, EH26 0QB, UK

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Correspondence to: E. Personne (erwan@bcgn.grignon.inra.fr)

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Abstract

A new biophysical model SURFATM-NH₃, simulating the ammonia (NH₃) exchange between terrestrial ecosystems and the atmosphere is presented. SURFATM-NH₃ consists of two coupled models: (i) an energy budget model and (ii) a pollutant exchange model, which distinguish the soil and plant exchange processes. The model describes the exchanges in terms of adsorption to leaf cuticles and bi-directional transport through leaf stomata and soil. The results of the model are compared with the flux measurements over grassland during the GRAMINAE Integrated Experiment at Braunschweig, Germany. The dataset of GRAMINAE allows the model to be tested in various climatic and agronomic conditions: prior to cutting, after cutting and then after the application of mineral fertilizer. The whole comparison shows close agreement between model and measurements for energy budget and ammonia fluxes. The major controls on the soil and plant emission potential are the physicochemical parameters for liquid-gas exchanges which are integrated in the compensation points for live leaves, litter and the soil surface. Modelled fluxes are highly sensitive to soil and plant surface temperatures, highlighting the importance of accurate estimates of these terms. The model suggests that the net flux depends not only on the foliar (stomatal) compensation point but also that of leaf litter. SURFATM-NH₃ represents a comprehensive approach to studying pollutant exchanges and its link with plant and soil functioning. It also provides a simplified generalised approach (SVAT model) applicable for atmospheric transport models.

1 Introduction

The exchange of trace gases and vapour pressure between terrestrial ecosystem and atmosphere is a key process the Earth's Biosphere functioning: at the local, regional and global scale, these exchanges participate in element cycling, influencing ecosystem productivity and background pollution. With the exception of CO₂, the exchange

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of trace gases (e.g., NH₃, O₃, SO₂, N₂O) at the surface is often included in mesoscale transport models or global scale models using a dry deposition velocity approach (Fowler et al., 1989; Wesely, 1989; Tulet et al., 2000) or emission factors (Li et al., 2001; Freibauer, 2003; Hyde et al., 2003), although recent studies use improved process based models (Grunhage and Haenel, 1997; Polcher et al., 1998; Ganzeveld et al., 2002; Nikolov and Zeller, 2003; Pinder et al., 2004; Theobald et al., 2004). In this context, this paper concentrates on atmospheric ammonia (NH₃) as a reference pollutant for the conception of exchange schemes of soil-plant-atmosphere interface that can be integrated at the lower-boundary conditions in global scale models or in mesoscale transport models.

Indeed, atmospheric ammonia (NH₃) mainly originates from agriculture (Bouwman et al., 1997; Anderson et al., 2003; Sutton et al., 2007; Zhang et al., 2008), of which animal waste is the main source (Van der Hoek, 1998; Zhang et al., 2008). Ammonia deposition leads to acidification and eutrophication of semi-natural ecosystems (Van Breemen and Van Dijk, 1988; Fangmeier et al., 1994; Dragosits et al., 2002) and to decrease of the plant biodiversity (Bobbink, 1991; Krupa, 2003; Stevens et al., 2004, 2006). The concentrations of NH₃ in the environment are generally in the range 0.1 to 5 µg m⁻³ NH₃ and can reach several tens of µg m⁻³ NH₃ in the vicinity of strong sources (Sutton et al., 1998b; Loubet et al., 2001). As a major constituent of the plant metabolism, NH₃ can either be absorbed or emitted by the vegetation (Sutton et al., 1993; Schjoerring et al., 2000). The bi-directional nature of NH₃ exchange between the atmosphere and the surface has been demonstrated in many studies (Farquhar et al., 1980; Erisman and Wyers, 1993; Sutton et al., 1995, 1998a).

However, the NH₃ flux above a canopy results from the combination of sources and sinks within the canopy, as emphasised by Nemitz et al. (2000a). In a grassland canopy the litter may be a strong source of NH₃ as suggested by laboratory studies (Husted and Schjoerring, 1995; Mattsson and Schjoerring, 2002, 2003), but the stomata could also release NH₃ following fertilisation (Husted et al., 2000; Loubet et al., 2002). However, the contribution of each compartment to the net flux is still not clear.

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Modelling NH_3 exchange has proven to be a good mean to interpret measured NH_3 fluxes at the canopy scale, and especially to evaluate the contribution of each canopy compartment to the net flux (e.g. Nemitz et al., 2000b). However, NH_3 emissions from the ground surface or from plants is known to depend exponentially on temperature, due to thermodynamic equilibria (e.g. Schjoerring, 1997), and stomatal resistance as any other gases (Sutton et al., 1993). Hence the NH_3 exchange model needs to correctly simulate the surface temperature of emitting or absorbing compartments (stomata and litter/soil surface) as well as the stomatal resistance.

In this paper, we present a bi-directional two-layer resistance model for heat and NH_3 , parameterised for a grassland canopy. The model SURFATM- NH_3 combines a resistive approach for the energy balance and for the NH_3 exchange. It incorporates an NH_3 stomatal compensation point as well as a litter or soil NH_3 compensation point, and a cuticular pathway. SURFATM- NH_3 model is then evaluated against measured fluxes of energy, water and ammonia, during the GRAMINAE Integrated Experiment above managed grassland at Braunschweig, Germany (Sutton et al., 2008).

2 Model description

SURFATM- NH_3 is a one-dimensional, bi-directional model, which simulates the latent (λE) and sensible (H) heat fluxes, as well as the NH_3 fluxes between the biogenic surfaces and the atmosphere. SURFATM- NH_3 is a resistance analogue model treating separately the vegetation layer and the soil layer (Monteith and Unsworth, 1990; Nemitz et al., 2001). SURFATM- NH_3 couples the energy balance of Choudhury and Monteith (1988), slightly modified (Appendix A), and the two-layer bi-directional NH_3 exchange model of Nemitz et al. (2000b). The model includes a stomatal compensation point for NH_3 (χ_s), and a cuticular resistance of foliage (R_{wf}^x), which are modelled following Husted et al. (2000) and Nemitz et al. (2000a). It also includes a soil/litter compensation point concentration (χ_{surf}) which allows ground based NH_3 emissions to be reproduced. The SURFATM- NH_3 model is based on the same resistive scheme for

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the energy balance and the NH₃ exchange and so with the same transfer resistances (aerodynamic, boundary layer, and stomatal) modulus the scalar diffusivities. The NH₃ exchange is directly coupled to the energy balance via the leaf temperature (T_{z_0}) and the surface temperature (T_{surf}), and the humidity in the canopy (e_{z_0}), which determine

5 χ_s , χ_{surf} , and R_{wf}^χ , respectively. Figure 1 shows the resistance analogue scheme for the heat, water vapour and NH₃ transfer.

2.1 Aerodynamic, boundary layer, stomatal, soil and “cuticular” resistances

In the following, the exponent or index i refers to either water vapour or NH₃. The diffusivity of NH₃ in air, D_{NH_3} , and the diffusivity for water vapour in air, D_w , are taken
10 as $D_{\text{NH}_3}=2.29 \text{ m}^2 \text{ s}^{-1}$ and $D_w=2.49 \text{ m}^2 \text{ s}^{-1}$ (Massman, 1998).

Aerodynamic resistances. The usual hypothesis is made of similarity between turbulent transfers of scalars, hence the aerodynamic resistances R_a and R_{ac} are supposed identical for water vapour, heat and NH₃ (details given in Appendix B).

Boundary layer resistances. Following Shuttleworth and Wallace (1985) and Choudhury and Monteith (1988), the canopy boundary layer resistances (R_{bf}^i , where i stands for scalar i), are expressed as a function of the leaf boundary layer resistance and wind speed inside the canopy:

$$R_{bf}^i = \left(\frac{D_i}{D_w}\right)^{-2/3} \cdot \frac{\alpha_u}{2 \cdot a \cdot \text{LAI}_{ss}} \cdot \left(\frac{\text{LW}}{u(h_c)}\right)^{1/2} \cdot \left[1 - \exp\left(-\frac{\alpha_u}{2}\right)\right]^{-1} \quad (1)$$

where LAI_{ss} is the leaf area index (single sided projected foliage surface), a is a coefficient equal to $0.01 \text{ s m}^{-1/2}$ (Choudhury and Montheith, 1988), α_u is defined by $u(z)=u(h_c) \cdot \exp[\alpha_u(z/h_c-1)]$, where $u(z)$ is the wind speed at height z , and h_c is the canopy height, LW is the characteristic width of a the leaves (m), and D_i and D_H are the diffusivities of the scalar i and heat, respectively. The ground surface boundary layer resistance is modelled following Hicks et al. (1987), integrating here an additional
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resistance (R_{litter}) for transfer due to the litter laying the soil surface:

$$R_{\text{bss}}^i = \frac{2}{\kappa \cdot u_{\text{ground}}^*} \cdot \left(\frac{Sc_i}{Pr} \right)^{2/3} + R_{\text{litter}} \quad (2)$$

where Sc_i is the Schmidt number for the scalar i ($Sc_i = \nu_a / D_i$, D_i being the diffusivity of the scalar i and ν_a the cinematic viscosity of air), Pr is the Prandtl number, and u_{ground}^* is the friction velocity near the soil surface, which is calculated following Loubet et al. (2006):

$$u_{\text{ground}}^* = \left((u^*)^2 \cdot \exp \left(1.2 \times LAI_{ss} \times \left(\frac{z_{0s}}{h_c} - 1 \right) \right) \right)^{1/2} \quad (3)$$

where z_{0s} is the ground surface roughness length, R_{litter} is an additional resistance, which is fixed at either 2000 s m^{-1} in order to simulate the transfer through the litter (from soil surface to the top of the litter) or 5000 s m^{-1} in order to take into account the closed stomata of the dead leaves over the soil (Jones, 1992).

Resistance parameterisation for NH_3 . For the component of transfer where turbulence is small by comparison with the diffusive processes (Fig. 1), NH_3 molecular diffusivity D_{NH_3} must be considered. Based on Eqs. (1) and (2), the diffusivity ratio $\mathfrak{R}_{\text{NH}_3}$ is used to define the NH_3 boundary resistances for soil and vegetation ($R_{\text{bss}}^{\text{NH}_3}$ and $R_{\text{bf}}^{\text{NH}_3}$). $\mathfrak{R}_{\text{NH}_3}$ varies with temperature (Massman, 1998) and is given as:

$$\mathfrak{R}_{\text{NH}_3} = \frac{D_{\text{NH}_3}}{D_w} = 0.92 \quad \text{at } 25^\circ\text{C} \quad (4)$$

Hence, the model takes into account these effects in the boundary layers resistances:

$$\begin{cases} R_{\text{bf}}^{\text{NH}_3} = \left(\mathfrak{R}_{\text{NH}_3} \right)^{-2/3} \cdot R_{\text{bf}} \\ R_{\text{bss}}^{\text{NH}_3} = \left(\mathfrak{R}_{\text{NH}_3} \right)^{-2/3} \cdot R_{\text{bss}} \end{cases} \quad (5)$$

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Stomatal resistance. The stomatal resistance for a gas compound i (R_s^i) is calculated following Jarvis (1976), as a function of the photosynthetically active radiation (PAR), and stress functions, with the parameterisation of Pleijel et al. (2004) (Appendix C).

Soil resistances. Following Choudhury and Monteith (1988), the dry and wet soil layer resistances for heat conduction are calculated as:

$$R_{\text{dry_soil}}^H = \rho_a \cdot c_p \cdot \frac{\Delta_{\text{dry}}}{\kappa_{\text{dry}}} \quad (6)$$

$$R_{\text{wet_soil}}^H = \rho_a \cdot c_p \cdot \frac{\Delta_{\text{wet}}}{\kappa_{\text{wet}}} \quad (7)$$

where κ is the thermal conductivity, c_p specific heat capacity of air, ρ_a the air density and the thickness of each layer. The subscripts wet and dry stands for the wet and the dry layer, respectively.

For the gas transfer in the soil, the soil resistance is evaluated according to the dry soil thickness Δ_{dry} with the following resistance:

$$R_{\text{dry_soil}}^i = \frac{\tau_{\text{soil}} \cdot \Delta_{\text{dry}}}{\rho \cdot D_i} \quad (8)$$

where ρ is the porosity of the soil, τ_{soil} is a tortuosity factor.

Cuticular resistance. For a simplified approach, cuticular exchanges for water are supposed to be negligible compared with stomatal exchange, while for NH₃, the resistance is parameterised without taking into account the chemical reactions with the surface. Hence in SURFATM-NH₃, the surface concentration χ_{wf} is assumed to be zero with the resistance depending on microclimate. Following Sutton et al. (1993) and Sutton et al. (1995), cuticular resistance is set to $R_{wf}^{\text{NH}_3}$ vary according to air relative humidity (RH in %). The parameterisation of Milford et al. (2001a) is used here because the agronomic conditions of their studies are similar to that at the Braunschweig grassland

(Sutton et al., 2001; Milford et al., 2001a):

$$R_{wf}^{\text{NH}_3} = R_{wf_min}^{\text{NH}_3} \cdot \exp\left(\frac{100 - \text{RH}}{7}\right) \quad (9)$$

where RH is the relative humidity, and $R_{wf_min}^{\text{NH}_3} = 30 \text{ s m}^{-1}$.

2.2 Sub-stomatal cavity and soil surface/litter NH_3 concentration

- 5 Following Schjoerring et al. (1998), the compensation point is modelled as resulting from the thermodynamic equilibrium between NH_3 in the liquid and in the gas phase as well as the acid-base equilibrium between NH_4^+ and NH_3 in the liquid phase:

$$\chi_i = K_{HA} \cdot K_{AC} \cdot \exp\left(\frac{\Delta H_{HA}^0 + \Delta H_{AC}^0}{R} \cdot \left(\frac{1}{298.15} - \frac{1}{T_i^K}\right)\right) \cdot \Gamma_i \quad (10)$$

10 where K_{HA} and K_{AC} are equilibrium constants at 25°C , and ΔH^0 are free enthalpies, R is the perfect gas constant, T^K is the temperature in Kelvin, and Γ is the emission potential. Subscripts HA and AC stand for “Henry” and “dissociation”, respectively; while subscript i designs the compartment considered : the sub-stomatal cavity (s), the interface between wet and dry soil (soil), or the ground surface/litter (surf). The temperatures have the corresponding subscript, except for the sub-stomatal cavity where the temperature $T_s = T_{20}$. The compensation point (χ_i) varies according to the temperature T_i and Γ_i , where Γ_i is the non-dimensional ratio $[\text{NH}_4^+]/[\text{H}^+]$, where brackets denote concentrations in mol mol^{-1} of available compound (not bound to soil colloids or leaf cells). Concerning the emission potential for the stomatal pathway, Γ_s can in some instances be estimated from measurements of $[\text{NH}_4^+]$ and the pH of the plant apoplast, or it can represent an adjustment parameter in fitting the model to measured fluxes. 15 in the literature, estimates of Γ_s are typically in the range 60–5800 (e.g., Loubet et al., 2002; Mattsson et al., 2008a, b), with the value of Γ_s being governed by N-cycling and

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plant metabolism (Riedo et al., 2002). In the model scheme used here (Fig. 1), concerning the soil pathway, Γ_{surf} can either be the emission potential of the soil surface or that of the litter or dead leaves lying on the ground Γ_{litter} , while Γ_{soil} is the emission potential at the dry-wet interface in the soil. Various models have examined the contributions of fertilisation, the soil water status, the microbiological activity and this “soil compensation point” (Genermont et al., 1998; Pinder et al., 2004). In the following, Γ_i will be computed from measured $[\text{NH}_4^+]$ and $[\text{H}^+]$.

2.3 Soil water balance

The evolution of the soil water balance is based on a two-layer approach where the soil evaporation leads to a drying of the upper dry layer, and to an increase of the thickness of this dry layer (Δ_{dry}) according to Choudhury and Montheith (1988). The plants are supposed to take up the water in the wet soil only. Hence the transpiration decreases the soil water content of the wet soil and hence the water availability for plants.

2.4 Operational of the model

SURFATM-NH₃ requires input data of concentration at the reference height, meteorology, soil and vegetation stand structure. Meteorological forcing includes values of air temperature (T_a), relative humidity (RH), net radiation (Rn) and, wind speed (u) at a reference height z_{ref} and precipitation (Rain). Soil water content is described by the field capacity (θ_{cc}), wilting point (θ_{wp}) and dry soil humidity (θ_{HA}) in order to define the soil water availability for plants. The single sided leaf area index (LAI_{ss}) and the height of the canopy (h_c) define the vegetation stand structure. The model is performed with quarter-hourly time-step.

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3 Material and methods

3.1 Experimental data

The energy balance model was validated against measurements performed over a grassland field. And the modelled NH_3 exchange is compared to NH_3 flux and concentration measurement performed at the same time. The dataset used is briefly described in this section.

The European project GRAMINAE (Grassland Ammonia Interactions Across Europe – Sutton et al., 2002, 2008) was instigated to quantify exchange of NH_3 with grasslands across an East-West transect across Europe. As part of this effort, an integrated experimental campaign took place 18 May–15 June 2000 at a 6.4 ha experimental agricultural grassland of the German Federal Agricultural Research Centre Braunschweig, Völkenrode (52°18' N, 10°26' E; 79 m a.s.l.).

Agronomic conditions in the experiment are described by Sutton et al. (2008) and show a large range of situations to evaluate the model: a) the vegetation was at first tall and dense; b) it was cut on 29 May 2000, and then left for 7 days; and c) the field was fertilized on 6 June with 108 kg N ha⁻¹ as calcium ammonium nitrate. The calendar events are summarized in Fig. 2. During the measurement period before the cut, the canopy height h_c increased from 0.65 to 0.75 m with a single sided leaf area index (LAI_{ss}) of 3.1 m² m⁻². After the cut, h_c and LAI_{ss} were 0.07 m and 0.3 m² m⁻² and developed up to 0.32 m and 1.4 m² m⁻² by 15 June.

The model is performed with quarter-hourly time-step in order to take into account the fast changes of surface temperature and energy fluxes and the hypothesis of the stationarity of the climatic data on this time-step (Lumley and Panofsky, 1964). Climatic data of the experimental site (Nemitz et al., 2008), provided inputs for T_a , RH, R_n , u and Rain, with the other input parameters used for the simulations summarized in Table 1. Model input included the atmospheric mean ammonia concentrations, χ_a , as estimated by Milford et al. (2008). Moreover, leaf (T'_{z0}), ground/litter (T_{surf}) and soil (T_{soil})

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temperatures were estimated from measured temperature in the canopy litter and soil with fine thermocouples.

3.2 Evaluation of heat balance model

As discussed in Nemitz et al. (2008), the measured heat fluxes lead to a lack of closure of the energy balance ($R_n = H + \lambda E + G$ + lack), by about 30%. However, since the model is based on the energy closure, the heat fluxes H and λE were adjusted so that $H + \lambda E = R_n - G$. Based on the arguments of Twine et al. (2000), the bowen ratio was maintained and both H and λE were increased by 29% (Nemitz et al., 2008). The canopy height h_c , and the leaf area index were prescribed from measurements. The measured and modelled H , λE , G , T_{z0} and T_{surf} are compared against each other for estimating the validity of the heat model.

3.3 Parameterisation of the NH_3 emission potentials Γ_s , Γ_{soil} and Γ_{litter}

The model inputs for Γ_s and Γ_{soil} were derived from plant and soil measurements made during the experiment, which also provided estimates for plant litter (Γ_{litter}). The measurements of apoplastic, litter and soil $[\text{NH}_4^+]$ and pH are described by Mattsson et al. (2008a), Herrmann et al. (2008), and Sutton et al. (2008), with the synthesis of the different values reported by Sutton et al. (2008). Based on this synthesis, we interpolated the measured values to provide simplified profiles of Γ_s , Γ_{soil} and Γ_{litter} through the experiment (Fig. 3). The huge range of measured values between Γ_s , Γ_{soil} and Γ_{litter} is apparent in Fig. 3. Γ_s values were rather modest, between 100–600, with an increase occurring after fertilization. Values of Γ_{soil} were much larger, especially after fertilization, indicating the ground surface as the dominant emission pathway for this period. It is notable, however, that Γ_{litter} values were very high in comparison with the values of Γ_s and Γ_{soil} , both before and after the cut, while after fertilization Γ_{litter} increased further, possibly due to the presence of fertilizer ammonium adsorbing to the litter.

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The interpolated lines in Fig. 1 provided the input Γ values for the model simulations, using two different approaches, named scenario S1 and scenario S2. In the first approach (S1), the ground surface emission was parameterised using the measured values of Γ_{soil} , with hypothesis that the NH₃ comes from the boundary between wet and dry soil (level soil in Fig. 3). Therefore, the value of Γ_{soil} was associated with the temperature at this level (T_{soil}^*) and the soil resistance (R_{soil}). In the second approach (S2), the ground surface emission was parameterised using the measured values of Γ_{litter} , with the hypothesis that the associated temperature is that of the soil surface (T_{SS} - level surf in Fig. 1), with the stomata of the litter assumed to be inactive providing an additional resistance $R_{\text{litter}}=5000 \text{ s m}^{-1}$ in the simulation.

In both approaches, the modelled Γ_s is used to estimate the sub-stomatal cavity NH₃ concentration χ_s using based on Eq. (8).

4 Results

The simulations of SURFATM-NH₃ were compared with the detailed energy balance measurements reported by Nemitz et al. (2008) and with the measured mean NH₃ fluxes determined by aerodynamic gradient method, as reported by Milford et al. (2008), including appropriate corrections for advection where necessary (Loubet et al., 2008). For certain days there was significant uncertainty in the mean fluxes, so that Milford et al. (2008) also reported an “alternative estimate” of the flux. Further comparison with flux measurements using a surface dispersion model (Loubet et al., 2007) and relaxed eddy accumulation (Hensen et al., 2008), provided independent data to distinguish the most robust flux estimates for these uncertain days (Sutton et al., 2008). The synthesized flux dataset was thus used for comparison with the model flux estimates of SURFATM-NH₃.

4.1 Energy budget

No calibrations were used for the part of the model which treats the energy budget. Figure 4 represents the various fluxes of the energy budget. The corrections of Twine et al. (2000), accounting for fluctuation methods and direct measurements of R_n , were applied and allow a coherent energy budget to be estimated with independent measurements of H and λE : the model shows a close agreement to the measured fluxes throughout the comparison (Table 2). A major change in fluxes magnitude occurs from the 29 May. The grassland cut led increased the total heat flux (H) and the soil heat conduction (G). This clear change is not observed for the modelled latent heat flux (λE) on 29 May, and may result from a transient increase in evaporation and drying of the grass cuttings prior to their removal.

4.2 Temperature

The modelled surface temperature of the soil and the foliage are the equilibrium variables of the energy budget. These variables are the key-connections between the energy budget and the ammonia exchange. Figure 5 shows the results of measured and modelled temperatures before and after the cut. The modelled soil surface and leaf temperature (T_{surf} and $T_{z0'}$) are higher than the air temperature (T_a) during the day, and vice versa during the night: the cooling and warming process of the canopy surfaces seems to be in good agreement with the measurements. During the day, the vegetation temperature is ranged between the measurements of the top and the bottom of the canopy. The agreement between the model and the measurements is within 2.5°C for $T_{z0'}$, and so the foliage temperature and 4°C for T_{surf} , the soil surface temperature. The worst agreement is just following the cut where the difference between measured and modelled temperatures reaches 4°C for $T_{z0'}$ and 10°C for T_{surf} . However before the cut, the agreement is much better 1°C for $T_{z0'}$ and 2°C for T_{surf} . It can be underline that these differences are smaller than the difference between the measured air and surface temperature which raise 5 to 7°C for the difference ($T_a - T_{z0'}$) and 10 to 15°C

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for the difference ($T_a - T_{\text{litter}}$)

4.3 Ammonia fluxes and dynamics of the emission potential

Figure 6 presents the comparison between modelled total NH_3 fluxes and the measured NH_3 fluxes above the field. From 21 to 29 May (before the cut), the NH_3 exchanges ranged between a deposition of $-50 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$ to an emission of $+40 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$. Following cutting, NH_3 emissions increased up to up to $500 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$ (Fig. 6). These emissions are an order of magnitude greater than the typical emission observed over the grassland previous to cutting. Following fertilization on 6 June, the fluxes immediately increased up to $2000 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$. These high emission values continued few days before progressively decreasing to similar emission fluxes prior to fertilization at daytime maxima near $500 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$. The typical diurnal pattern of emission fluxes after the cut and the fertilisation typically exhibited a clear increase in emission starting at 06:00 UT and reverting to near zero at 20:00 UT (Fig. 6).

The simulations are based on two scenarios: the soil emission scenario (S1) and the litter emission scenario (S2). Both the simulations using litter and soil emissions reproduce the diurnal dynamics of emissions. Prior to the cut, the temporal dynamics of both models are similar, with the litter model most close to the absolute value of the measurements. The two scenarios reproduce satisfactorily the fluxes before the cut (with a tendency for the model to give more emissions periods than the measurements) as well as a week after fertilisation (with higher modelled emissions at nights). The two scenario however fail to reproduce the pulse of emission the day of the cut (29 May). Moreover, the two scenarios show deposition the 28 May between 06:00 UT and 12:00 UT, while the measurements show small emissions, possibly denoting a local advection episode (Loubet et al., 2006).

After cutting and before fertilisation, the soil scenario (S1) tend to underestimate the NH_3 emissions by roughly 66%, while the litter emission scenario (S2) tend to

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overestimates it by roughly 30%, except on the 1 June, where it correctly predicted the fluxes.

SURFATM-NH₃ clearly simulates the increase in NH₃ emission following cutting using both the litter and soil emission parameterisations. It may be noted from Fig. 3 (bioassay Gammas) that the parameterised Γ_{soil} was unchanged following cutting. Therefore, the increased NH₃ emissions in the soil source simulation are a result of other factors, primarily the removal of the overlying canopy (which would recapture a fraction of the ground surface emission) and the warmer ground temperatures (Fig. 5). However, the modelled soil source (S1) does not generally explain all the increase in NH₃ fluxes observed during this period (apart from 30–31 May). The larger emissions on 1–4 June are more closely simulated using the litter NH₃ source (S2), including the larger values on 3 June.

For the post-fertilization period, both the soil source and litter source parameterisations (S1 and S2) demonstrate the further increase in NH₃ emission, which is closely coupled to the changing measured values of Γ_{soil} , Γ_{litter} over this period (Fig. 3). It is notable that the simulation using the soil source parameterisation does not reproduce the initial emission after fertilization on 5 June, since measured soil [NH₄⁺] only increased on 6–7 June, which may reflect sampling uncertainty, linked also with soil sampling depth over the layer 0–10 cm. Conversely, the litter parameterisation (S2) over estimates emissions on 8–10 June, while both parameterisations reveal the subsequent decrease in emissions on 11–14 June.

In details during the two days following fertilisation, the soil emission scenario show almost no NH₃ emissions, while the litter emission scenario reproduces fairly well the magnitude and the pattern of the fluxes (especially the night time emissions during the nights 5–6 June and 6–7 June). Following the pattern of Γ_{soil} (Fig. 3), three days after fertilisation, the soil emission scenario start to give larger NH₃ emissions, but still smaller than the measured ones, while the litter emission scenario agree very well with measured NH₃ fluxes. From day 4 to day 6 after fertilisation, the soil emission scenario gives better agreement with measured NH₃ fluxes than the litter emission scenario

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which overestimates the fluxes both during nights and during days.

5 Discussions

The close agreement for H , λE and G fluxes (Fig. 4) between measurements and simulations ensures a consistent calibration for the physical and biological parameters (Table 1). It can be supposed that the values used for the stomatal resistance and soil thermal conductivities are well adapted to the experimental site. The correction of Twine et al. (2000) was used to have a closing measured energy budget. However, without Twine's corrections the modelled latent heat flux (λE) is overestimated by 26%, while the modelled sensible heat flux (H) is only overestimated by 11%, hence suggesting that the measured λE was probably underestimated, which confirms the analysis of Nemitz et al. (2008).

The litter is taken into account in the resistance scheme of the energy balance model with an additional resistance (R_{litter}). This litter layer reduces the transfer of sensible heat between the soil and the canopy (larger R_{drysoil}^H) and reduces G , which was overestimated by the model at night by 28%. The additional "litter" resistance of 2000 s m^{-1} almost decreases the difference between modelled and measured G at night. The litter would also induce an additional water "reservoir" in the canopy which would lead to evaporation during the day and condensation at night, hence modifying the energy partition at the ground (Tuzet et al., 1993).

The modelled canopy temperature $T_{z0'}$ is close to the measured top green leaves, by less than 2°C , which is smaller than the difference between the measured T_a and $T_{z0'}$ (Fig. 5). The soil surface temperature T_{surf} is also well modelled except for three days following the cut, where it reaches 3 to 6°C above the measured T_{surf} . This overestimation is certainly linked with the presence of the grass left on the field (striming in Fig. 2), which would have increase the resistance for heat transfer at the ground surface.

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5.1 Uncertainty in stomatal resistance and emission potential

The good agreement between the modelled and measured heat fluxes and temperatures also implies that the stomatal resistance R_s^W , $R_s^{NH_3}$ and the canopy temperatures ($T_{z0'}$ and T_{surf} , respectively), and humidity are all correctly predicted. This is without questioning the Twine et al. (2000) correction which drastically changes R_s . A new parameterisation should multiply R_s^W by two in order to reproduce the range of the latent heat flux directly measured, without correction.

An increase of 100% of the stomatal resistance increases the heat exchanges and increases the gap between model and measurements by 18% for the heat fluxes H and 2% for the soil heat conduction G while this variation for the stomatal resistance induces a decrease of 25% for the latent heat flux λE . Such variation of the stomatal resistance induces only a small change of the temperature smaller than 0.5°C . The uncertainty on R_s based on the error of H , λE and G induces a small effect on the surface temperatures

The temperatures $T_{z0'}$ and T_{surf} are very sensitive parameters of the NH_3 exchange model since the compensation points χ_s and χ_{surf} are exponentially dependent to temperature (Eq. 8). The coupling between the energy balance model and the pollutant exchange model is essentially made via $T_{z0'}$ and T_{surf} . Hence the fact that these two modelled temperatures are in agreement with the measured ones within 2°C (in general), implies a potential error on χ_s and χ_{surf} of 20%.

5.2 Dynamic of the exchanges

Examining the period prior to the cut (Fig. 6a), NH_3 fluxes are lower than $100\text{ ng m}^{-2}\text{ s}^{-1}$ and deposition was predominant. This deposition would have been governed by the plant exchanges according to the covering foliage of plant ($LAI_{ss}=3$). Similar fluxes have been reported elsewhere for managed grassland (Milford et al., 2001a) and as in our experiment, deposition fluxes are close to $50\text{ ng NH}_3\text{ m}^{-2}\text{ s}^{-1}$. In these conditions of deposition, when vegetation is dense, the model is sensitive to the parameterisation

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of the cuticular deposition. For ammonia, air water content (expressed as relative humidity or vapour pressure) is a determinant variable, and in this simplified approach based on the parameterisation of Milford et al. (2001b), only this variable is sufficient to reproduce much of the pattern in deposition. In fact, this approach is simple and operational with only climatic forcing (RH at the reference height z_{ref}), but does not reproduce NH_3 desorption processes (Sutton et al., 1998a; Flechard et al., 1999) or specific microclimate in the vicinity of the foliage. However it remains consistent for the model because this approach is validated for various conditions and plant surface types (van Hove et al., 1989; Sutton et al., 1995; Nemitz et al., 2001). The first improvement could be simply done by using the relative humidity of the air in the vicinity of the foliage (at the level z_0') instead of the air ambient RH on condition that the parameterisation of Milford et al. (2001a) remains adapted to this change of compartment level (z_0' instead of z_{ref}). The cuticular exchanges could also be treated in a dynamical approach, as an electric capacitor with a surface charge χ_{wf} , which may be released under certain conditions (Sutton et al., 1998b). The exchange conditions are related to the surface chemical processes, the air vapour pressure and the temperatures, and to the climatic events (rainfall and surface leaching) (Flechard et al., 1999). The potential importance of these cuticular adsorption/desorption processes for the Braunschweig dataset are investigated by Burkhardt et al. (2008).

After the vegetation is cut, the role of the ground surface exchange enhances, as does the influence of the ground surface temperature. The role of ground temperature was particularly important during the period after cutting where soil surface temperature increased by $15^\circ C$ during the day in comparison with values at night.

The ammonia exchanges from plant were parameterised by values of emission potential ranged between 100–600 (Fig. 3), which are typical of other similar measurements (e.g., Loubet et al., 2002). For the soil emission following N fertilisation, the simple linear decrease from a maximum value of $\Gamma_{soil}=300\ 000$ to a value of 40 000 ten days after N-fertilisation gives a reasonable agreement provided the maximum value for the NH_3 fluxes is well adjusted. In a more detailed analysis, the decrease of this soil

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emission potential should be take into account the degradation on the soil surface and the dilution or leaching with water soil in order to have an improvement of the simulated results in comparison with measurements, and these aspects should be considered in future work. This result demonstrates the influence of the agronomic/soil management and the link between the microclimate and the pollutant exchange. Similarly, while overall agreement was found between the model and the measurements, as well as the results of parallel cuvette measurements (David et al., 2008), the measured Γ_{soil} and Γ_{litter} values must also be considered as uncertain. For example, mineralization of NH_4^+ in litter may be considered will depend on moisture availability, so that loss of NH_3 to the atmosphere will deplete Γ_{litter} values substantially until more mineralization is able to occur. Such dynamics, not included in the present simulation can easily explain the differences between model and measurements that were observed.

5.3 Partition of NH_3 fluxes between the soil, the litter and the stomata

Baring in mind that Γ_s , Γ_{soil} and Γ_{litter} were prescribed, the model with the litter scenario agrees very well with the measurements over a period which shows a change two order of magnitude of the NH_3 flux (Fig. 6). The only hypothesis made were that the litter had an additional resistance $R_{\text{litter}}=5000 \text{ s m}^{-1}$ of the order of closed stomata (Jones, 1992; Weyers and Meidner, 1990), and that the bulk solution of the leaves was in equilibrium with the atmosphere, which implies that the NH_4^+ measured in the bulk extracts is freely available, and that the bulk pH is representative of that solution. The good agreement between the model and the measurements allows to investigate the origin of the flux with the model:

Before the cut. The good agreement at the transition from uncut to cut grassland, with a constant $\Gamma_{\text{litter}}/\Gamma_{\text{soil}}$ (Fig. 3), and the fact that both scenario agree quite well before the cut shows that before the cut, the stomata are absorbing most of the NH_3 emitted from the ground. The model shows that between 5 and 20 $\text{ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$ are emitted from the ground before the cut but that the flux above the canopy is a mean deposition flux

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of $-5 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$ due to vegetation absorption (Fig. 7). However, the ground NH_3 emissions still have a great impact on the overall NH_3 exchange by increasing the NH_3 concentration around the leaves. Based on the model, if there was no source at the ground before the cut, the NH_3 flux within the canopy would be a deposition flux of 5 to $40 \text{ ng NH}_3 \text{ m}^{-2} \text{ s}^{-1}$. The fact that the soil scenario (S1) shows a slight offset in the predicted flux before the cut probably indicates an overestimation of the litter resistance during that period.

After the cut. The NH_3 fluxes increase following the cut (Fig. 6). There is some discussion in the recent literature about whether the cut would increase the stomatal compensation point as a result of remobilisation (David et al., 2008). However, Loubet et al. (2002) have found no increase in Γ_s immediately following the cut but a slight increase later. Moreover the levels of Γ_s in Loubet et al. (2002) were comparable to the Γ_s found in this study and they can not explain the levels of emissions found after the cut. The fact that the measured NH_3 fluxes lie between the litter emission scenario and the soil emission scenario strongly suggests that the source of NH_3 emission following the cut is the ground. The increased NH_3 emissions following the cut can be explained by two factors: (i) the weight of the stomatal sink is reduced by the cut, and (ii) the temperature of the litter/soil changes from a daily mean of $15 \pm 10^\circ\text{C}$ before the cut to a daily mean of $20 \pm 15^\circ\text{C}$ after the cut (Fig. 5). Baring in mind that a 5°C increase of the surface emitting NH_3 induces a twofold increase in emissions (Eq. 10), this means that following the cut, the maximum emission from the litter is multiplied by 8, which is what is observed in Fig. 7. The fact that the litter emission scenario (S2) agrees better with the measurements than the soil emission scenario (S1) can be explained by the soil temperature being roughly $2\text{--}3^\circ\text{C}$ smaller than the litter temperature. This is clear on the 31 May, where the soil temperature is 5°C smaller than the litter temperature and the soil emission scenario gives NH_3 emissions twice as small as the litter emission scenario.

However, the litter emission scenario tends to overestimates the NH_3 fluxes following the cut (by 18%). This overestimation might be due to (i) the exchange process

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at the litter being not a perfect equilibrium as expressed in Eq. (8), (ii) the Γ_{litter} being overestimated by the extraction technique, (iii) the soil surface temperature being overestimated by the model during that period, (iv) an underestimation of the litter resistance, (v) the progressive transfer of the ammonium from the litter to the soil, or (vi) the cuticular exchange which could be higher than modelled in this study. Although all these hypotheses are plausible, they can not be proven with the available data.

After the fertilisation. The fertilisation induces an increases of the NH_3 fluxes which is well reproduced by the model (Fig. 6) due to the Γ_{litter} increasing just following the application of fertiliser (and two days later Γ_{soil} increases also). The NH_3 emissions during the night between the 5 and the 6 June and the 6 and the 7 June is typical of non-stomatal emissions and is well reproduces by the litter emission scenario. The soil emission scenario gives deposition NH_3 fluxes the 5 and 6 June, which shows that $\chi_{z0} < \chi_a(z_{\text{ref}})$ (Fig. 1), hence demonstrating that the soil emission scenario (Γ_{soil} , and R_{litter}) fails to reproduce the emissions with the observed increase of NH_3 concentration. However, the soil emission scenario gives progressively increasing NH_3 emissions and matches the measured emissions six days following the fertilisation, while in the same period, the litter emission scenario gives too large emissions. Hence the simulations shown in Fig. 6 suggest that the main source following fertilisation is the litter which has effectively received the ammonium-nitrate pellets, and which contain the water (due to condensation) necessary for dissolving these pellets. However, the overestimation of the litter scenario in the following days (8 to 10 June) is still unclear. It might be due to (i) the litter temperature being overestimated by the model (Fig. 5) (ii) the litter resistance R_{litter} changing due to either a migration of NH_4^+ to the bottom of the litter, or (iii) NH_4^+ being not freely available due to metabolic changes.

6 Conclusions

The energy balance model presented in this study is shown to be adapted for modelling the latent and sensible heat fluxes over a grassland successively cut and fertilised,

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based on the prescription of measured canopy height and leaf area index. The model also succeeds in simulating the leaf and ground surfaces temperatures.

The overall agreement between the energy balance model and the measurements implies that the stomatal resistance is correctly modelled. The correct predictions of temperatures and stomatal resistance validates the coupling between the energy balance model and the NH_3 exchange model, since NH_3 exchange is mainly influenced by the stomatal resistance and the surface concentration which is exponentially linked to the temperature.

Using measured emission potentials of the apoplasm and the litter, the NH_3 exchange model successfully simulates the measured NH_3 fluxes during the cut and fertilisation period, over which the fluxes changes by two order of magnitude. The analysis of the partitioning of the fluxes between the model compartments, especially before and after the cut shows that the grassland can be described as the superposition of a litter/soil surface source and a stomatal sink. Of the different compensation points simulated, i.e. for green leaves, litter and the soil surface, the classical role of a foliar compensation point is rather different in the present study. Here, instead of the net flux depending on the balance of the air concentration and the foliar (stomatal) compensation point, the overall canopy compensation point and net fluxes are influenced to a large degree by emission potentials from the leaf litter. Prior to the cut, these emissions are mostly recaptured by the overlaying canopy, while they dominate net emissions following cutting and fertilization. Future work should thus pay more attention to the dynamics of nitrogen cycling with conditions at the litter and soil surface.

The agreement between the modelled and measured NH_3 fluxes hence demonstrate (i) the necessity to consider two layers (stomata and litter/soil surface), (ii) the need to couple with an energy balance model which can simulate the leaf and litter/soil surface temperature, and (iii) the interests in using NH_3 emissions potentials in the litter and the apoplasm, which can be measured in the field.

The latter point also shows the limit of this model which needs the emissions potentials of the apoplasm and the stomata to be prescribed, as well as the canopy height

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and leaf area index. This emphasises the need to improve our understanding of the seasonal pattern of these emissions potential, which implies a better understanding of the ammonium metabolism and pH regulation in the litter as well as the apoplasm of growing leaves, and their interaction with the soil.

5 Overall, the well behaviour of the coupled SURFATM-NH₃ provides a basis that is also suited for application to other gaseous compounds. This model thus provides a simplified generalised approach for application to atmospheric transport modelling.

Appendix A

10 Description of the energy balance model

Radiation, heat and vapour transfer. The net absorption of radiation by the vegetation and the soil Rn_T is given by (Varlet-Grancher et al., 1989; Tuzet and Perrier, 1992):

$$Rn_T = Rn_{veg} + Rn_{soil} \quad (A1)$$

$$Rn_{veg} = Rn_T \cdot \exp(-k_{Rn} \cdot LAI) \quad (A2)$$

15 The energy received by the leaves is partitioned between latent and sensible heat components, while at the soil surface, an additional conduction heat flux is included:

$$Rn_{veg} = H_{veg} + \lambda E_{veg} \quad (A3)$$

$$Rn_{soil} = H_{soil} + \lambda E_{soil} + G \quad (A4)$$

The total heat flux H_T , and the total latent heat flux λE_T are calculated as:

$$20 H_T = \rho_a \cdot c_p \cdot \frac{T_a - T_{z0}}{R_a} \quad (A5)$$

$$\lambda E_T = \frac{\rho_a \cdot c_p}{\gamma} \cdot \frac{e_a - e_{z0}}{R_a} \quad (A6)$$

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In the canopy, the flux partition is given by:

$$H_{\text{veg}} = \rho_a \cdot c_p \cdot \frac{T_{z0} - T_{z0'}}{R_{bf}^H} \quad (\text{A7})$$

$$\lambda E_{\text{veg}} = \frac{\rho_a \cdot c_p}{\gamma} \cdot \frac{e_{z0} - e_{z0'}}{R_{bf}^W} = \frac{\rho_a \cdot c_p}{\gamma} \cdot \frac{e_{z0} - e_s^*}{R_{bf}^W + R_{sf}^W} \quad (\text{A8})$$

At the soil surface, the heat fluxes are given by:

$$H_s = \rho_a \cdot c_p \cdot \frac{T_{z0} - T_{\text{surf}}}{R_{bss}^H + R_{ac}} \quad (\text{A9})$$

$$\lambda E_s = \frac{\rho_a \cdot c_p}{\gamma} \cdot \frac{e_{z0} - e_{\text{surf}}}{R_{bss}^W + R_{ac}} = \frac{\rho_a \cdot c_p}{\gamma} \cdot \frac{e_{z0} - e_{\text{soil}}^*}{R_{bss}^W + R_{ac} + R_{\text{dry_soil}}^W} \quad (\text{A10})$$

$$G = \lambda_{\text{wet}} \cdot \frac{T_{\text{bot}} - T_{\text{soil}}}{\Delta_{\text{wet}}} = \rho_a \cdot c_p \cdot \frac{T_{\text{bot}} - T_{\text{soil}}}{R_{\text{wet_soil}}^H} \quad (\text{A11})$$

As in Choudhury and Monteith (1988), the volumetric heat capacity for air in Eq. (A11) appears for algebraic convenience (λ_{wet} is the thermal conductivity extending from the soil bottom to the soil wet-dry boundary, over a thickness Δ_{wet}). The resolution of the energy budget, which involves iterations to account for buoyancy, is performed with the method proposed by Choudhury and Monteith (1988).

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Appendix B

Details of the aerodynamic resistances

Aerodynamic resistance above the canopy. The aerodynamic resistance for scalar above the canopy (R_a), at height z_{ref} , is calculated as:

$$R_a = \frac{1}{\kappa^2 \cdot u(Z)} \cdot \left\{ \ln \left[\frac{Z}{z_0} \right] - \Psi_H(Z/L) \right\} \left\{ \ln \left[\frac{Z}{z_0} \right] - \Psi_M(Z/L) \right\} \quad (\text{B1})$$

where κ is the Von-Kàrmàn constant (0.4), $Z = z_{\text{ref}} - d$, d being the displacement height, $u(Z)$ is the wind speed, z_0 is the canopy roughness height, L is the Monin-Obukhov length, and Ψ_H and Ψ_M are the stability correction functions for heat and momentum, respectively. The correction functions of Dyers and Hicks (1970) are used.

Aerodynamic resistance inside the canopy. Considering that the foliage has a homogeneous vertically distribution, the windspeed decreases exponentially (Cowan, 1965):

$$u(z) = u(h_c) \cdot \exp \left[\alpha_u \cdot \left(\frac{z}{h_c} - 1 \right) \right] \quad (\text{B2})$$

with $u(z)$, the wind speed inside the canopy at height z , $u(h_c)$ the wind speed at the canopy height (h_c), α_u is the attenuation coefficient for the decrease of the wind speed inside the cover (Raupach et al., 1996). With the hypothesis that the decrease of the diffusivity is proportional to the decrease of the wind speed inside the canopy, the aerodynamic resistance inside the cover (R_{ac}) takes the form:

$$R_{ac} = \frac{h_c \cdot \exp(\alpha_u)}{\alpha_w \cdot K_M(h_c)} \cdot \left\{ \exp(-\alpha_u \cdot z_{0s} \cdot h_c) - \exp \left(\frac{-\alpha_u(d + z_0)}{h_c} \right) \right\} \quad (\text{B3})$$

where $K_M(h_c)$ is the eddy diffusivity coefficient at canopy height h_c , and z_{0s} is the ground surface roughness length.

For more exact analysis, some corrections can be integrated if standard deviation of the vertical wind speed can be measured or modelled (Raupach, 1989).

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Details of the stomatal resistance model.

Following Pleijel and al (2004), the stomatal conductance for the gas i g_s^i per leaf are
is calculated as:

$$g_s^i = \frac{D_i}{D_w} \max \{g_{\min}; g_{\max} (g_{VPD} \cdot g_T \cdot g_{PAR} \cdot g_{SWP} \cdot g_{\text{time}})\} \quad (C1)$$

where D_i and D_w are the molecular diffusivities of the gas i and of water vapour in air, respectively; g_{\min} and g_{\max} denote, respectively, the minimum and maximum stomatal conductance allowed for a certain species by the model. The factors g_{VPD} , g_T , g_{PAR} and g_{time} represent the short-term effects of leaf-to-air vapour pressure difference, leaf temperature, photosynthetically active radiation and time of day. The influence of time-of-day is an effect of the internal water potential of the plant (Livingston and Black, 1987). The effect of soil water potential is reflected by the g_{SWP} factor. Although at very high concentrations NH_3 can have an effect on stomata aperture (van Hove et al., 1989), at normal ambient concentrations this effect is expected to be minimal. So, no effect of ammonia on g_s^i is included in the present implementation of the model. As the fluxes from foliage surface integrate the exchanges from the individual leaves, the canopy stomatal resistance for water is estimated as:

$$R_s^W = (\overline{g_s})^{-1} = \left(\int_0^{\text{LAI}} (g_s^W) \cdot d\text{LAI}' \right)^{-1} \quad (C2)$$

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References

- Anderson, N., Strader, R., and Davidson, C.: Airborne reduced nitrogen: ammonia emissions from agriculture and other sources, *Environ. Int.*, 29, 277–286, 2003.
- Bates, R. G. and Pinching, G. D.: Dissociation constant of aqueous ammonia at 0 to 50 °C from m.f studies of the ammonium salt of a weak acid, *Am. Chem. Soc. J.*, 72, 1393–1396, 1950.
- Bobbink, R.: Effect of nutrient enrichment in Dutch chalk grassland, *J. Appl. Ecol.*, 28, 28–41, 1991.
- Bouwman, A. F., Lee, D. S., Asman, W. A. H., Dentener, F. J., and van der Hoek, K. W.: A global high-resolution emission inventory for ammonia, *Global Biogeochem. Cy.*, 11, 561–587, 1997.
- Burkhardt, J., Flechard, C. R., Gressens, F., Mattsson, M., Jongejan, P. A. C., Erisman, J. W., Weidinger, T., Meszaros, R., Nemitz, E., and Sutton, M. A.: Modeling the dynamic chemical interactions of atmospheric ammonia and other trace gases with measured leaf surface wetness in a managed grassland canopy, *Biogeosciences Discuss.*, 5, 2505–2539, 2008, <http://www.biogeosciences-discuss.net/5/2505/2008/>.
- Carsel, R. F. and Parrish, R. S.: Developing joint probability distributions of soil water retention characteristics, *Water Resour. Res.*, 24, 755–769, 1988.
- Choudhury, B. J. and Monteith, J. L.: A four-layer model for the heat budget of homogeneous land surfaces, *Q. J. Roy. Meteor. Soc.*, 114, 373–398, 1988.
- Cowan, I. R.: Transport of water in soil plant atmosphere system, *J. Appl. Ecol.*, 2, 221–239, 1965.
- David, M., Loubet, B., Cellier, P., Mattsson, M., Schjoerring, J. K., Nemitz, E., Roche, R., Riedo, M., and Sutton M. A.: Ammonia sources and sinks in an intensively managed grassland using dynamic chambers, *Biogeosciences Discuss.*, submitted, 2008.
- David, M., Roche, R., Mattsson, M., Sutton, M. A., Dämmgen, U., Schjoerring, J. K., and Cellier, P.: The effects of management on ammonia fluxes over a grassland using dynamic chambers, *Biogeosciences Discuss.*, submitted, 2008.
- Dragosits, U., Theobald, M. R., Place, C. J., Lord, E., Webb, J., Hill, J., ApSimon, H. M., and Sutton, M. A.: Ammonia, emission, deposition and impact assessments at the field scale: a case of study of sub-grid spatial variability, *Environ. Pollut.*, 117, 147–158, 2002.
- Dyers, A. G. and Hicks, B. B.: Flux-profile relationship in the constant flux layer, *Q. J. Roy. Meteor. Soc.*, 96, 715–721, 1970.

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Erismann, J. W., and Wyers, G. P.: Continuous measurements of surface exchange of SO₂ and NH₃ : implications for their possible interaction in the deposition process, *Atmos. Environ.*, 27, 1937–1949, 1993.

Fangmeier, A., Hadwiger-Fangmeier, A., Van der Eerden, L., and Jäger, H. J.: Effects of atmospheric ammonia on vegetation – a review, *Environ. Pollut.*, 86, 43–82, 1994.

Farquhar, G. D., Firth, P. M., Wetselaar, R., and Wier, B.: On the gaseous exchange of ammonia between leaves and the environment: determination of the ammonia compensation point, *Plant Physiol.*, 66, 710–714, 1980.

Flechard, C., Fowler, D., Sutton, M. A., and Cape J. N.: Modelling of ammonia and sulphur dioxide exchange over moorland vegetation, *Q. J. Roy. Meteor. Soc.*, 125, 2611–2641, 1999.

Fowler, D., Cape, J. N., and Unsworth, M. H.: Deposition of atmospheric pollutants on forest, *Phil. Trans. Roy. Soc. London B.*, 324, 247–265, 1989.

Freibauer, A.: Regionalised inventory of biogenic greenhouse gas emissions from European agriculture, *Eur. J. Agron.*, 19, 153–160, 2003.

Ganzeveld, L. N., Lelieveld, J., Dentener, F. J., Krol, M. C., and Roelofs, G.-J.: Atmosphere-biosphere trace gas exchanges simulated with a single-column model, *J. Geophys. Res.*, 107(D16), 4297, doi:10.1029/2001JD000684, 2002.

Genermont, S., Cellier, P., Flura, D., Morvan, T., and Laville, P.: Measuring ammonia fluxes after slurry spreading under actual field conditions, *Atmos. Environ.*, 32, 279–284, 1998.

Grünhage, L. and Haenel, H.-D.: PLATIN (PLant-ATmosphere-Interaction) I : A model of plant-atmosphere interaction for estimating absorbed doses of gaseous air pollutants, *Environ. Pollut.*, 98, 37–50, 1997.

Guyot G.: *Physics of the Environment and Climate*. John Wiley, Chichester, 632 pp., 1998.

Hensen, A., Nemitz, E., Flynn, M., Blatter, A., Jones, S. K., Sørensen, L. L., Hensen, B., Pryor, S., Jensen, B., Otjes, R. P., Cobussen, J., Loubet, B., Erismann, J. W., Gallagher, M. W., Nefftel, A., and Sutton, M. A.: Inter-comparison of ammonia fluxes obtained using the Relaxed Eddy Accumulation technique, *Biogeosciences Discuss.*, submitted, 2008.

Herrmann, B., Mattsson, M., Jones, S. K., Cellier, P., Milford, C., Sutton, M. A., Schjoerring, J. K., and Nefftel, A.: Vertical structure and diurnal variability of ammonia exchange potential within an intensively managed grass canopy, *Biogeosciences Discuss.*, 5, 2897–2921, 2008, <http://www.biogeosciences-discuss.net/5/2897/2008/>.

Hicks, B. B., Baldocchi, D. D., Meyers, T. P., Hosker Jr., R. P., and Matt, D. R.: A preliminary multiple resistance routine for deriving dry deposition velocities from measured quantities,

BGD

6, 71–114, 2009

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- Water Air Soil. Poll., 36, 311–330, 1987.
- Husted, S. and Schjorerring, J. K.: Apoplastic pH and ammonium concentration in leaves of *Brassica napus* L., *Plant Physiol.*, 109, 1453–1460, 1995.
- Husted, S., Schjorerring, J. K., Nielsen, K. H., Nemitz, E., and Sutton, M. A.: Stomatal compensation points for ammonia in oilseed rape plants under field conditions, *Agr. Forest. Meteorol.*, 105, 371–383, 2000.
- Hyde, B. P., Carton, O. T., O’Toole, P., and Misselbrook, T. H.: A new inventory of ammonia emissions from Irish agriculture, *Atmos. Environ.*, 37, 55–62, 2003.
- Jarvis, P. G.: The interpretation of the variation in leaf water potential and stomatal conductance found in canopies in the field, *Phil. Trans. Roy. Soc. London. B*, 273, 375–391, 1976
- Jones, H. G.: *Plants and Microclimate. A Quantitative Approach to Environmental Plant Physiology*, Cambridge University Press, 428 pp., 1992.
- Krupa, S. V.: Effects of ammonia (NH₃) on terrestrial vegetation: a review, *Environ. Pollut.*, 124, 179–221, 2003.
- Li, C., Zhuang, Y., Cao, M., Crill, P., Frolking, S., Moore, B., Salas, W., Song, W., and Wang, X.: Comparing a process-based agro-system model to the IPCC methodology for developing a national inventory of N₂O emissions from arable lands in China, *Nutr. Cycl. Agrosys.*, 60, 159–175, 2001.
- Livingston, N. J. and Black, T. A.: Stomatal characteristics and transpiration of three species of conifer seedlings planted on a high elevation south-facing clear-cut, *Can. J. Forest Res.*, 17, 1273–1282, 1987.
- Loubet, B.: *Modélisation du dépôt sec d’ammoniac atmosphérique à proximité des sources*, Ph-D. Thésis, 329 pp., Paul Sabatier University, Toulouse, France, 2000.
- Loubet, B., Milford, C., Sutton, M. A., and Cellier, P.: Investigation of the interactions between sources and sinks of atmospheric ammonia in an upland landscape using a simplified dispersion exchange, *J. Geophys. Res.*, 106(D20), 24 183–24 195, 2001.
- Loubet, B., Milford, C., Hill, P. W., Tang, Y. S., Cellier, P., and Sutton, M. A.: Seasonal variability of apoplastic NH₄⁺ and pH in an intensively managed grassland, *Plant Soil*, 238, 97–110, 2002.
- Loubet, B., Cellier, P., Genermont, S., Laville, P., and Flura, D.: Measurement of short-range dispersion and deposition of ammonia over a maize canopy, *Agr. Forest Meteorol.*, 114, 175–196, 2003.
- Loubet, B., Cellier, P., Milford, and Sutton, M. A.: A coupled dispersion and exchange model

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for short-range dry deposition of atmospheric ammonia, Q. J. Roy. Meteor. Soc., 132, 1733–1763, 2006.

Loubet, B., Milford, C., Hensen, C., Dämmgen, U., Erisman, J. W., Cellier, P., and Sutton, M. A.: Advection of ammonia over a pasture field, and its effect on gradient flux measurements, Biogeosciences Discuss., submitted, 2008.

Lumley, J. L. and Panofsky, H. A.: The structure of Atmospheric Turbulence. Wiley-Interscience, New York, 239 pp., 1964.

Massman, W. J.: A review of the molecular diffusivities of H₂O, CO₂, CH₄, CO, O₃, SO₂, NH₃, N₂O, NO and NO₂ in air, O₂ and N₂ near STP, Atmos. Environ., 32, 1111–1127, 1998.

Mattsson, M. and Schjoerring, J. K.: Dynamic and steady-state responses of inorganic nitrogen pools and NH₃ exchange in leaves of Lolium perenne and Bromus erectus to changes in root nitrogen supply, Plant Physiol., 128, 742–750, 2002.

Mattsson, M. and Schjoerring, J. K.: Senescence-induced changes in apoplastic and bulk tissue ammonia concentrations of ryegrass leaves, New Phytol., 160, 489–499, 2003.

Mattsson, M., Herrmann, B., David, M., Loubet, B., Riedo, M., Theobald, M. R., Sutton, M. A., Bruhn, D., Neftel, A., and Schjoerring, J. K.: Temporal variability in bioassays of ammonia exchange potential in relation to plant and soil nitrogen parameters in intensively managed grassland, Biogeosciences Discuss., 5, 2749–2772, 2008a, <http://www.biogeosciences-discuss.net/5/2749/2008/>.

Mattsson, M., Herrmann, B., Jones, S. K., Neftel, A., Sutton, M. A., and Schjoerring, J. K.: Contribution of different grass species to plant-atmosphere ammonia exchange in intensively managed grassland, Biogeosciences Discuss., 5, 2583–2605, 2008b, <http://www.biogeosciences-discuss.net/5/2583/2008/>.

Milford, C., Theobald, M. R., Nemitz, E., and Sutton, M. A.: Dynamics of ammonia exchange in response to cutting and fertilizing in an intensively-managed grassland, Water Air Soil Poll., Focus, 1, 167–176, 2001a.

Milford, C., Theobald, M. R., Nemitz, E., and Sutton, M. A.: Dynamics of ammonia exchange in response to cutting and fertilising in an intensively-managed grassland, in: Air-Surface Exchange of Gases and Particles (2000), edited by: Fowler, D., Pitcairn, C. E. R., and Erisman, J.-W., Kluwer, Academic Publishers, 2001b.

Milford, C., Theobald, M. R., Nemitz, E., Hargreaves, K. J., Horvath, L., Raso, J., Dämmgen, U., Neftel, A., Jones, S. K., Hensen, A., Loubet, B., Cellier, P., and Sutton, M. A.: Ammonia fluxes in relation to cutting and fertilization of an intensively managed grassland derived from

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an inter-comparison of gradient measurements, *Biogeosciences Discuss.*, 5, 4699–4744, 2008,

<http://www.biogeosciences-discuss.net/5/4699/2008/>.

Monteith, J. L. and Unsworth, M. H.: *Principles of Environmental Physics*, 2nd edn., Arnold Press, London, 291 pp., 1990.

Nemitz, E., Sutton, M. A., Gut, A., San Jose, R., Husted, S., and Schjørring, J. K.: Sources and sinks of ammonia within an oilseed rape canopy, *Agr. Forest Meteorol.*, 105, 385–404, 2000a.

Nemitz, E., Sutton, M. A., Schjørring, J. K., Husted, S., and Wyers G. P.: Resistance modelling of ammonia exchange over oilseed rape, *Agr. Forest Meteorol.*, 105, 405–425, 2000b.

Nemitz, E., Milford, C., and Sutton M. A.: A two-layer canopy compensation point model for describing bi-directional biosphere/atmosphere exchange of ammonia, *Q. J. Roy. Meteor. Soc.*, 127, 815–833, 2001.

Nemitz, E., Hargreaves, K. J., Neftel, A., Loubet, B., Cellier, P., Dorsey, J. R., Flynn, M., Hensen, A., Weidinger, T., Meszaros, R., Horvath, L., Fruehauf, C., Sutton, M. A., and Gallagher, M. W.: Inter-comparison of measurements and assessment of the turbulent exchange and energy balance of an intensively managed grassland, *Biogeosciences Discussions*, submitted, 2008.

Nikolov, N. and Zeller, K.: Modeling coupled interactions of carbon, water and ozone exchange terrestrial ecosystems and atmosphere. I: Model description, *Environ. Pollut.*, 124, 231–246, 2003.

Pinder, R. W., Pekney, N. J., Davidson, C. I., and Adams, P. J.: A process-based model of ammonia emissions from dairy cows: improved temporal and spatial resolution, *Atmos. Environ.*, 38, 1357–1365, 2004

Pleijel, H., Danielsson, H., Ojanperä, K., De Temmerman, L., Högy, P., Badiani, M., and Karlsson, P. E.: Relationships between ozone exposure and yield loss in European wheat and potato – A comparison of concentration- and flux-based exposure indices, *Atmos. Environ.*, 38, 2259–2269, 2004.

Polcher, J., McAvaney, B., Viterbo, P., Gaertner, M.-A., Hahmann, A., Mahfouf, J.-F., Noilhan, J., Phillips, T., Pitman, A., Schlosser, C. A., Schulz, J.-P., Timbal, B., Versegny, D., and Xue, Y.: A proposal for a general interface between land-surface schemes and general circulation models, *Global Planet. Change*, 19, 261–276, 1998.

Raupach, M. R.: Stand overstorey processes, *Phil. Trans. Roy. Soc. London. B*, 324, 175–190,

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1989.

Raupach, M. R., Finnigan, J. J., and Brunet, Y.: Coherent eddies and turbulence inside vegetation canopies. The mixing layer analogy, *Bound.-Lay. Meteorol.*, 78, 351–382, 1996.

Schjoerring, J. K.: Plant-atmosphere ammonia exchange: Quantification, physiology regulation and interaction with environmental factors, D. Sc. Thesis, Roy. Veterinary and Agric. Univ. Copenhagen, Denmark, 55 pp., 1997.

Schjoerring, J. K., Husted, S., and Mattsson, M.: Physiological parameters controlling plant-atmosphere ammonia exchange, *Atmos. Environ.*, 32, 491–498, 1998.

Schjoerring, J. K., Husted, S., Mack, G., Nielsen, K. H., Finnemann, J., and Mattsson M.: Physiological regulation of plant-atmosphere ammonia exchange, *Plant Soil*, 221, 95–102, 2000.

Shuttleworth, W. J. and Wallace, S. J.: Evaporation from sparse crop – An energy combination theory, *Q. J. Roy. Meteor. Soc.*, 111, 477–507, 1985.

Stevens, C. J., Dise, N. B., Gowing, D. J. G., and Mountford, J. O.: Loss of forb diversity in relation to nitrogen deposition in the UK : regional trends and potential controls, *Glob. Change Biol.*, 12, 1823–1833, 2006.

Stevens, C. J., Dise, N. B., Mountford, J. O., and Gowing D. J. G.: Impact of nitrogen deposition on the species richness of grasslands, *Science*, 303, 1876–1879, 2004.

Sutton, M. A., Pitcairn, C. E. R., and Fowler, D.: The exchange of ammonia between the atmosphere and plant communities, *Adv. Ecol. Res.*, 24, 301–389, 1993.

Sutton, M. A., Schjoerring, J. K., and Wyer, G. P.: Plant atmosphere exchange of ammonia, *Phil. Trans. Roy. Soc. Lond. A.*, 351, 261–278, 1995.

Sutton, M. A., Burkardt, J. K., Guerin, D., Nemitz, E., and Fowler, D.: Development of resistance models to describe measurements of bi-directional ammonia surface atmosphere exchange, *Atmos. Environ.*, 32, 473–480, 1998a.

Sutton, M. A., Milford, C., Dragosits, U., Place, C. J., Singles, R. J., Smith, R. I., Pitcairn, C. E. R., Fowler, D., Hill, J., ApSimon, H. M., Ross, C., Hill, R., Jarvis, S. C., Pain, B. F., Phillips, V. C., Harrison, R., Moss, D., Webb, J., Espenhahn, S. E., Lee, D. S., Hornung, M., Ullyett, J., Bull, K. R., Emmett, B. A., Lowe, J., and Wyers, G. P.: Dispersion, deposition and impacts of atmospheric ammonia: quantifying local budgets and spatial variability, *Environ. Pollut.*, 102, 349–361, 1998b.

Sutton, M. A., Milford, C., Nemitz, E., Theobald, M. R., Hill, P. W., Fowler, D., Schjoerring, J. K., Mattsson, M., Nielsen, K.H., Husted, S., Erisman, J. W., Otjes, R., Hensen, A., Mosquera, J.,

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Sutton, M. A., Nemitz, E., Erisman, J. W., Beier C., Butterbach Bahl, K., Cellier, P., de Vries, W., Cotrufo, F., Skiba, U., Di Marco, C., Jones, S. K., Laville, P., Soussana, J-F, Loubet, B., Twigg, M., Famulari, D., Whitehead, J., Gallagher, M.W., Neftel, A., Flechard, C. R., Herrman, B., Calaca, P. L., Schjoerring, J. K., Daemmgen, U., Horvarth, L., Tang, Y. S., Emmett, B. A., Tietema, A., Penuelas, J., Kesik, M., Brüeggemann, N., Pilegaard, K., Vesala, T., Campbell, C. L., Olesen, J. E., Dragosits, U., Theobald, M. R., Levy, P., Mobbs, D. C., Milne, R., Viovy, N., Vuichard, N., Smith, J. U., Smith, P., Bergamaschi, P., Fowler, D., and Reis, S.: Challenges in quantifying biosphere-atmosphere exchange of nitrogen species, *Environ. Pollut.*, 150, 125–139, 2007.

Sutton, M. A., Nemitz, E., Theobald, M. R., Milford, C., Dorsey, J. R., Gallagher, M. W., Hensen, A., Jongejan, P. A. C., Erisman, J. W., Mattsson, M., Schjoerring, J. K., Cellier, P., Loubet, B., Roche, R., Neftel, A., Hermann, B., Jones, S. K., Lehmann, B. E., Horvath, L., Weidinger, T., Rajkai, K., Burkhardt, J., Löpmeier, F. J., and Daemmgen, U.: Dynamics of ammonia exchange with cut grassland: strategy and implementation of the GRAMINAE Integrated Experiment, *Biogeosciences Discuss.*, 5, 3347–3407, 2008, <http://www.biogeosciences-discuss.net/5/3347/2008/>.

Sutton, M. A., Nemitz, E., Theobald, M. R., Milford, C., Dorsey, J. R., Gallagher, M. W., Hensen, A., Jongejan, P. A. C., Erisman, J. W., Mattsson, M., Schjoerring, J. K., Cellier, P., Loubet, B., Roche, R., Neftel, A., Hermann, B., Jones, S. K., Lehmann, B. E., Horvath, L., Weidinger, T., Rajkai, K., Burkhardt, J., Lpmeier, F. J., and Daemmgen, U.: Dynamics of ammonia exchange with cut grassland: strategy and implementation of the GRAMINAE Integrated Experiment, *Biogeosciences Discuss.*, 5, 3347–3407, 2008, <http://www.biogeosciences-discuss.net/5/3347/2008/>.

Theobald, M. R., Dragosits, U., Place, C. J., Smith, J. U., Sozanska, M. Brown, L., Scholefield, D., Del Prado, A., Webb, A., Whitehead, P. G., Angus, A., Hodge, I. D., Fowler, D., and Sutton, M. A.: Modelling nitrogen fluxes at the landscape scale, *Water Air Soil Poll.*, 6, 135–142, 2004.

Tulet, P., Crassier, V., and Rosset R.: Air pollution modelling at a regional scale, *Environ. Modell.*

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Softw., 15, 693–701, 2000.

Tuzet, A. and Perrier, A.: Crop water budget estimation of irrigation requirement, ICID Bulletin, 44, 1–16, 1992.

Tuzet, A., Perrier, A., and Oulid Aissa, A. K.: A prediction model for field drying of hay using a heat balance method, Agr. Forest Meteorol., 65, 63–89, 1993.

Twine, T. E., Kustas, W. P., Noman, J. M., Cook, D. R., Houser, P. R., Meyers, T. P., Prueger, J. H., Starks, P. J., and Wesely, M. L.: Correcting eddy-covariance flux underestimates over a grassland, Agr. Forest Meteorol., 103, 279–300, 2000.

Van Breemen, N. and Van Dijk, H. F. G.: Ecosystem effects of atmospheric deposition of nitrogen in The Netherlands, Environ. Pollut., 54, 249–274, 1988.

Van der Hoek, K. W.: Estimating ammonia emission factors in Europe: summary of the work of the UNECE ammonia expert panel, Atmos. Environ., 32, 315–316, 1998.

Van Hove, L. W. A., Koops, A. J., Adema, E. H., Vredenberg, W. J., and Pieters, G. A.: A study of the adsorption of NH₃ and SO₂ on leaf surfaces, Atmos. Environ., 23, 1479–1486, 1989.

Varlet-Grancher, C., Gosse, G., Chartier, M., Sinoquet, H., Bonhomme, R., and Allirand, J.-M.: Mise au point: rayonnement solaire absorbé ou intercepté par un couvert végétal, Agronomie, 9, 419–439, 1989.

Weyers, J. D. B. and Meidner, H.: Methods in Stomatal Research, Longman Scientific and Technical edn., 1990.

Zhang, Y., Wu, S.-Y., Krishnan, S., Wang, K., Queen, A., Aneja, V. P., and Arya, S. P.: Modeling agricultural air quality: Current status, major challenges, and outlook, Atmos. Environ., 42, 3218–3237, 2008.

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Table 1. List of the input parameters used in the SURFATM-NH₃ model. The origin of the used values is indicated in the last column.

Physical Constants	Values (at 20 °C)	Reference	
ρ_a	density of air (20 °C)	1.19 (kg m ⁻³)	Monteith and Unsworth (1990)
c_p	Specific heat capacity of air	1010 (J kg ⁻¹ K ⁻¹)	Monteith and Unsworth (1990)
D_{air}	Air thermal diffusivity	2.22 10 ⁻⁵ (m ² s ⁻¹)	Monteith and Unsworth (1990)
D_{NH_3}	Molecular diffusion for NH ₃	2.29 10 ⁻⁵ (m ² s ⁻¹)	Massman (1998)
D_W	Molecular diffusion for vapour	2.49 10 ⁻⁵ (m ² s ⁻¹)	Massman (1998)
ν_a	Air cinematic viscosity (20 °C)	1.55 10 ⁻⁵ (m ² s ⁻¹)	Monteith and Unsworth (1990)
Pr	Prandtl number	0.71 (-)	Grunhage and Haenel (1997)
Sc ^{NH₃}	Schmidt number for NH ₃	0.92 (-)	Grunhage and Haenel (1997)
Chemical Constants			
K_{HA}	Henry Constant	10 ^{-3.14} (-)	Loubet (2000)
K_{AC}	Dissociation constant for acid-base dissociation NH ₄ ⁺ /NH ₃	10 ^{-9.25} (mol l ⁻¹)	Bates and Pinching (1953)
ΔH_{AC}^0	Free Enthalpy for acid-base dissociation NH ₄ ⁺ /NH ₃	52.21 (kJ mol ⁻¹)	Flecharad et al. (1999)
ΔH_{HA}^0	Free Enthalpy for NH ₃ volatilisation	34.18 (kJ mol ⁻¹)	Flecharad et al. (1999)
Physical Surface Parameters			
κ_{wet}	Thermal conductivity for wet soil	1.8 (W m ⁻¹ K ⁻¹)	Range [1.6; 2.2] Monteith and Unsworth (1990)
κ_{dry}	Thermal conductivity for dry soil	0.28 (W m ⁻¹ K ⁻¹)	Range [0.2; 0.3] Monteith and Unsworth (1990)
$\tau_{0,soil}$	Soil tortuosity	2.5 (-)	Choudhury and Monteith (1988)
p	Soil porosity	0.36 (-)	Estimated from measured soil saturation
σ_w	Attenuation coefficient for wind speed	4.2 (-)	Choudhury and Montheith (1988)
k_{Rn}	Radiation attenuation coefficient	0.65 (-)	Guyot (1998)
z_{soil}	Soil roughness	0.02 (m)	
z_0	Vegetation roughness	Calculated (m)	Tuzet et al. (1992)
d	Vegetation displacement displacement	Calculated (m)	Tuzet et al. (1992)
LW	Characteristic width of a the leaves	0.05 (m)	
h_c	Vegetation height	Measured (m)	0.07 m–0.76 m Sutton et al. (2002) and (2008)
LA _{l,ss}	Leaf Area Index single side	Measured	0.14–3.1 Sutton et al. (2002) and (2008)

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Table 2. Coefficients of the linear regressions for the comparisons model=f(measure) in terms of energy fluxes.

Whole period (22 May–15 June)	
<i>H</i>	$y=0.90x+17$ ($r^2=0.88$)
λE	$y=1.02x+6$ ($r^2=0.87$)
<i>G</i>	$y=0.72x-8$ ($r^2=0.85$)

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Table 3. Parameterisations used in the stomatal resistance model. All conductances are in m s^{-1} . PAR is the photosynthetically active radiation in ($\mu\text{mol m}^{-2} \text{s}^{-1}$), VPD is the leaf-to-air vapour pressure deficit (kPa), $T_{20'}$ is the canopy temperature ($^{\circ}\text{C}$), SWP is the soil water potential (MPa), time is the time of day is denoted (hh/24).

Name	Parameterisation	Comments	Units
g_{\max}	0.01	identical to	$407 \text{ mmol H}_2\text{O m}^{-2} \text{ s}^{-1}$
g_{PAR}	$\{1 - \exp(-0.012 \cdot \text{PAR})\}$	PAR in	$\mu\text{mol m}^{-2} \text{ s}^{-1}$
g_{VPD}	$\left\{1 + (\text{VPD}/2.7)^8\right\}^{-1}$	VPD in	kPa
g_T	If $T_{20'} < 27^{\circ}\text{C}$ then $g_T = \left\{(1 + (T/17)^{-10})^{-1}\right\} \times 1.01$ If $T_{20'} > 27^{\circ}\text{C}$ then $g_T = \left\{1 + (T/35)^{25}\right\}^{-1}$ If $\text{time} < 0.5$ $g_{\text{time}} = 1$	$T_{20'}$ is the canopy temperature in	$^{\circ}\text{C}$
g_{time}	If $\text{time} > 0.5$ $g_{\text{phen}} = \left\{1 + (\text{time}/0.72)^{15}\right\}^{-1}$	Time of day expressed in the equation as	h/24
g_{SWP}^*	If $\text{SWP} > -0.018$ then $g_{\text{SWP}} = 1$ If $\text{SWP} < -0.018$ then $g_{\text{SWP}} = 12 \cdot \text{SWP} + 1.2$	SWP is the soil water potential in	MPa

* the pedotransfer function of Carsel and Parrish (1988) is used to extrapolated soil water moisture to soil water potential.

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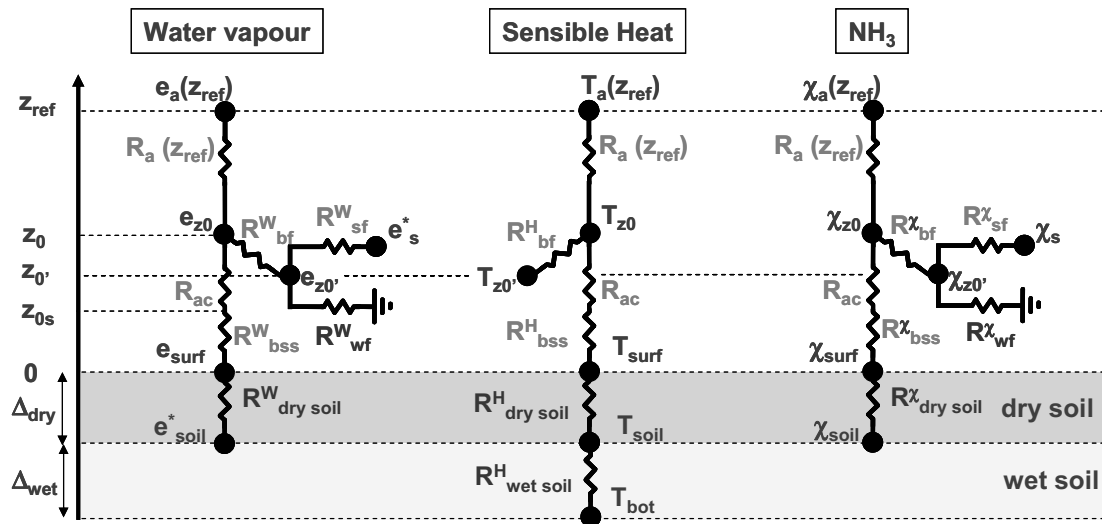


Fig. 1. Resistance scheme for water vapour, heat, and NH₃ exchange models. Where z is the height above ground; e , T and χ refer to the water vapour partial pressure, the temperature and the NH₃ concentration respectively; R_a , R_{ac} , R_{bf} , R_{bs} , $R_{drysoil}$, $R_{wetsoil}$, R_{sf} and R_{wf} are the aerodynamic resistance, the canopy aerodynamic resistance, the leaf boundary layer resistance, the soil boundary layer resistance, the soil dry resistance, the soil wet resistance, the stomatal resistance and the cuticular resistance, respectively; indexes ref, a, z₀, z₀', z_{0s}, s, surf, soil, and bot, refers to reference, atmospheric, canopy roughness height for momentum, canopy roughness height for scalars, soil roughness height, soil boundary, soil surface, dry/wet boundary in the soil, and bottom of the wet boundary in the soil, respectively, Δ_{dry} and Δ_{wet} are the heights of the dry and wet soil compartments, respectively.

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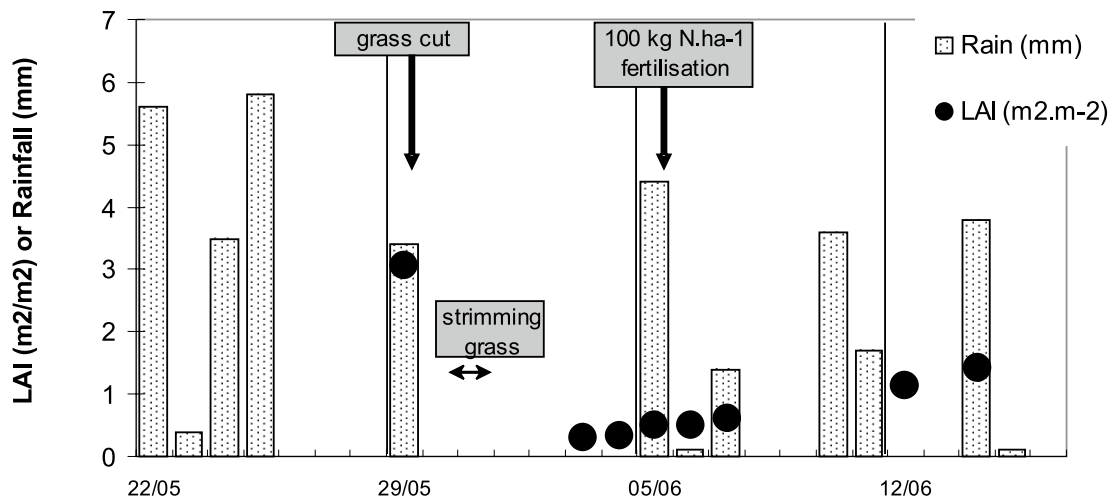


Fig. 2. Management, growth and rainfall during the GRAMINAE experiment. Rainfall is indicated by bars (in mm); LAI_{ss} measurements are reported in the figure by black points (in m² m⁻²); management events (cut, strimming and fertilisation) are indicated by arrows.

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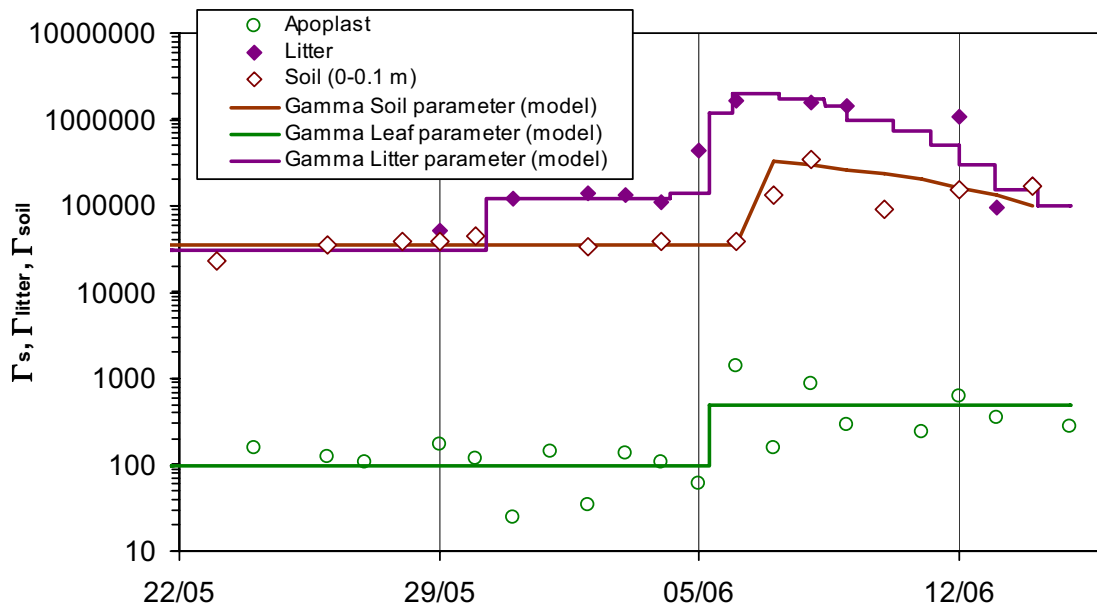


Fig. 3. Evolution of the emission potential for the soil (Γ_{soil}), the plant (Γ_s) and the litter (Γ_{litter}). Points results from measurements (Mattsson et al., 2008a,) and the continuous lines are the continuous values which are introduced for the simulations.

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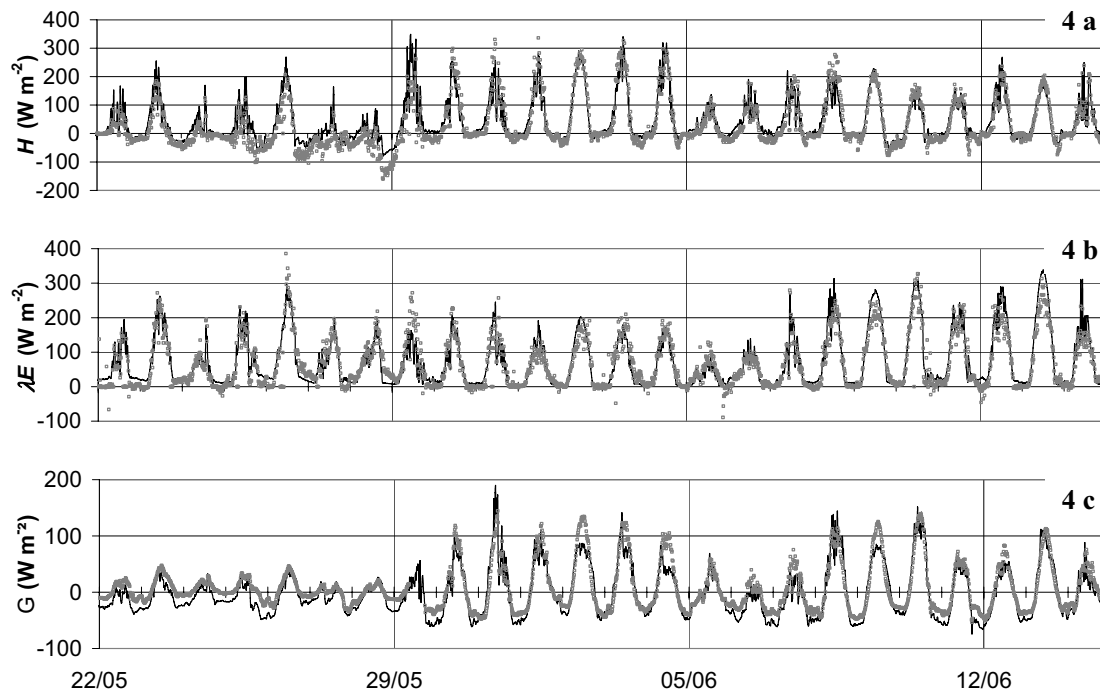


Fig. 4. Modelled (line) and measured (dots) **(a)** sensible heat flux H , **(b)** latent heat flux λE , and **(c)** soil heat flux G .

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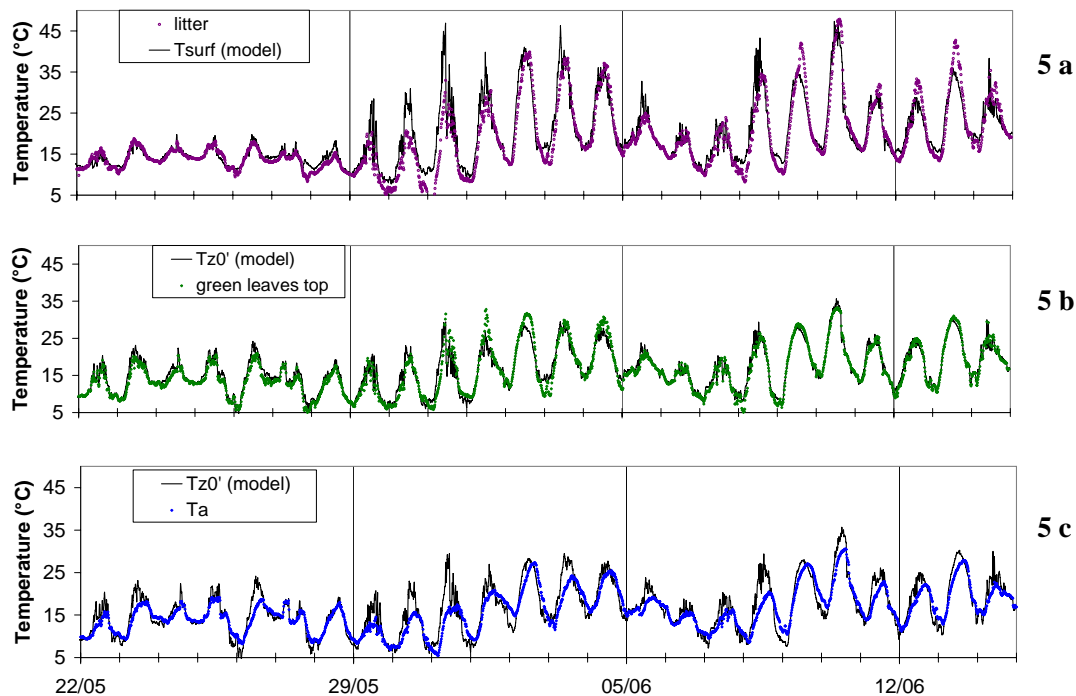


Fig. 5. Comparison of modelled (lines) and measured (dots) **(a)** ground surface temperature, and **(b)** canopy temperature. The measured air and canopy temperature are also shown in **(c)** for comparison.

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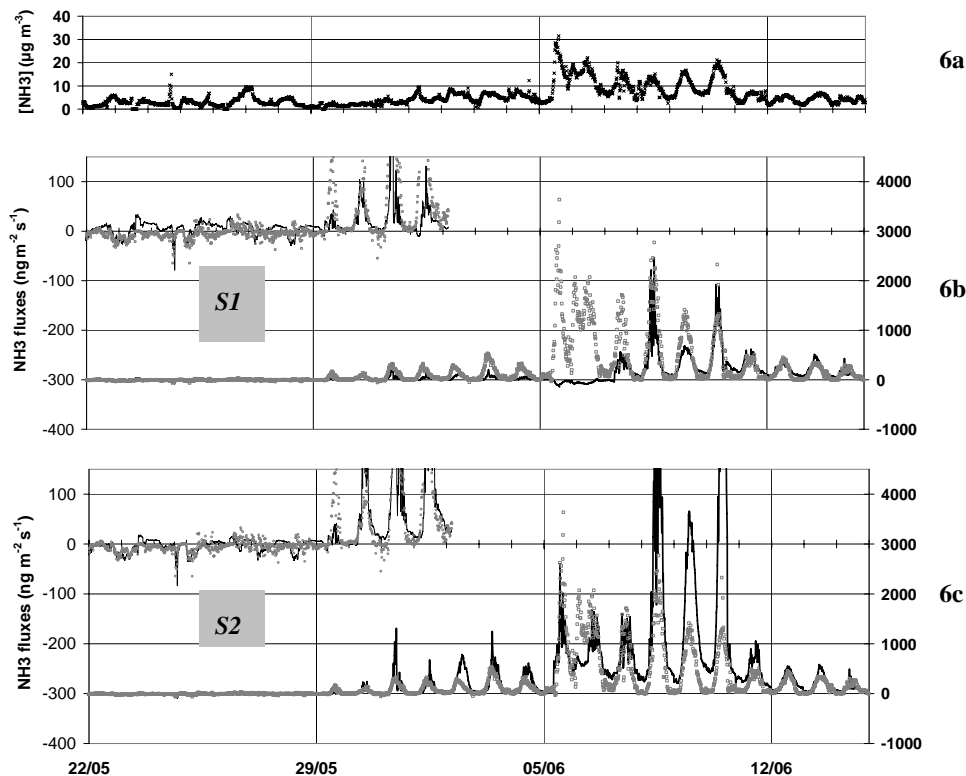


Fig. 6. Concentration of NH₃ measured at 1 m height (a). Modelled (lines) and measured (dots) NH₃ fluxes above the grassland field, based on the soil emission scenario S1 (b), and the litter emission scenario S2 (c). Note that there are two y-axis in order to magnify the period 21/05 to 31/05 (left y-axis), whereas the right axis applies for following period.

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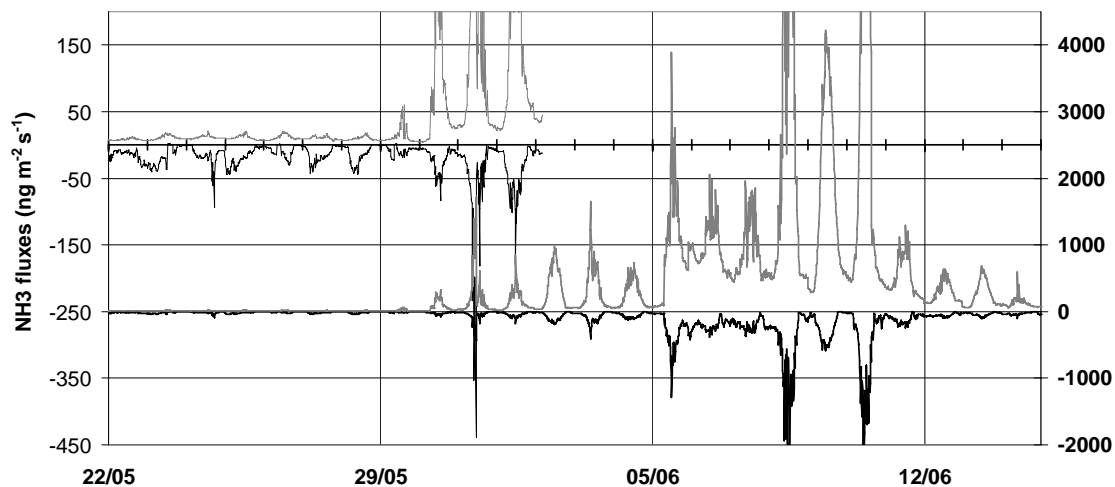


Fig. 7. Partition of the fluxes between the ground and the stomata, for the litter scenario *S2*. Grey line represents the exchange due to the litter and black line represents the exchange due to the vegetation.

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