Modelling ammonia deposition near large agricultural sources with a coupled Lagrangian Stochastic, k-ε, and diffusion resistance approach

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Outline

- The issue of NH_3 deposition near hot spots
- Challenges of measuring and modelling NH_3 deposition near hot spots
- A model coupling k-epsilon turbulence, Lagrangian Stochastic dispersion and resistance-based deposition
- Application to large feedlots in the USA
- Application to tree belt recapture systems in the UK
- Conclusion

The issue of NH_3 deposition near hot spots

Ammonia has strong environmental impacts

NH_3

Aerosol formation

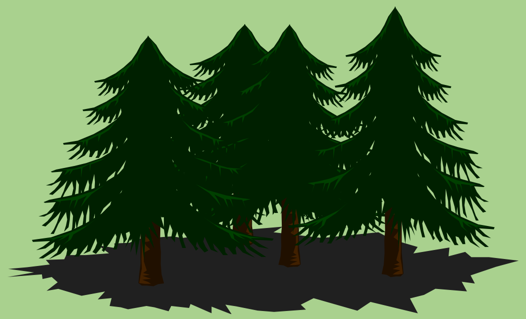
NH_4^+

NO_3^-

SO_4^{--}

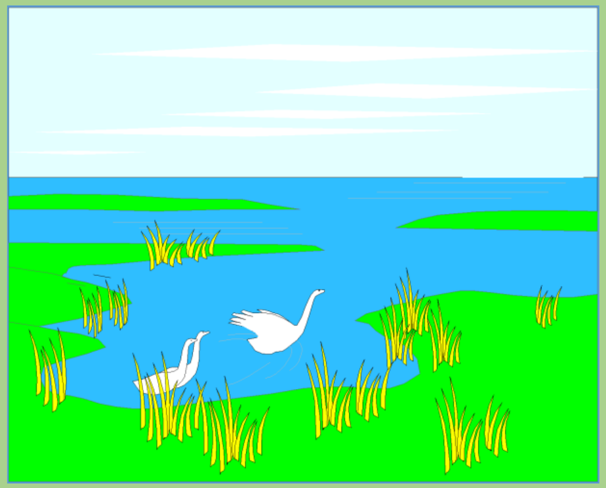
Cl^-

Acidification

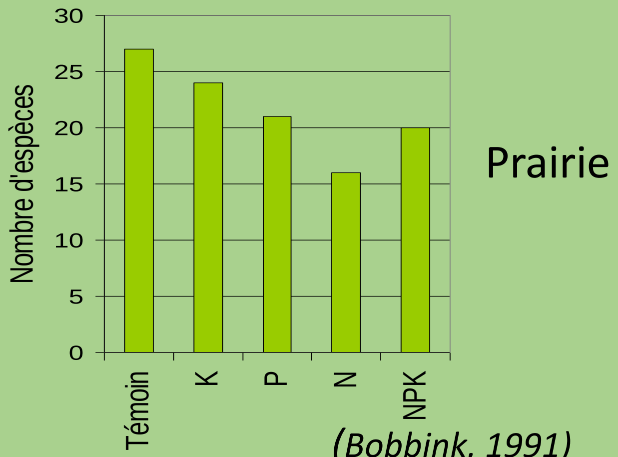


$NH_4^+ \rightarrow NO_3^- + 2H^+ + \ldots$

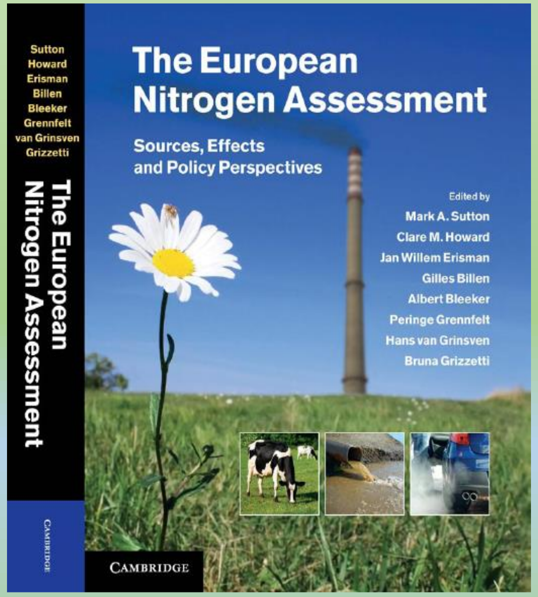
Eutrophication



Biodiversity loss



(Bobbink, 1991)



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van Grinsven
Grizzetti

The European Nitrogen Assessment

The European Nitrogen Assessment

Sources, Effects and Policy Perspectives

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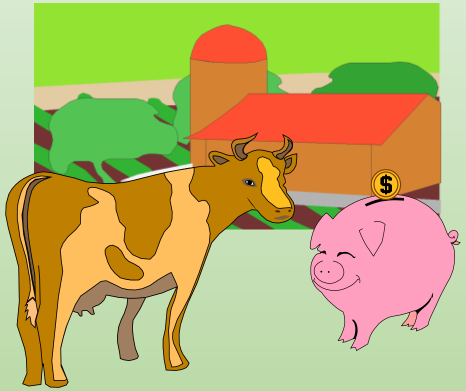
The issue of NH_3 deposition near hot spots

Hot spots are the dominant source of NH_3

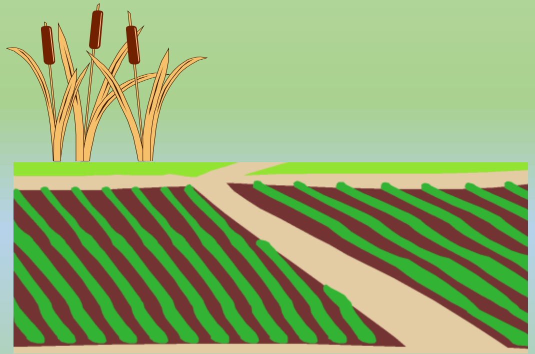
~60% of NH3 emissions in France is from animal farming (including application to the field)

https://www.citepa.org/fr/2022-nh3



Animal housings, manure storages

- Local in space
- Extended in time



Land spread manure

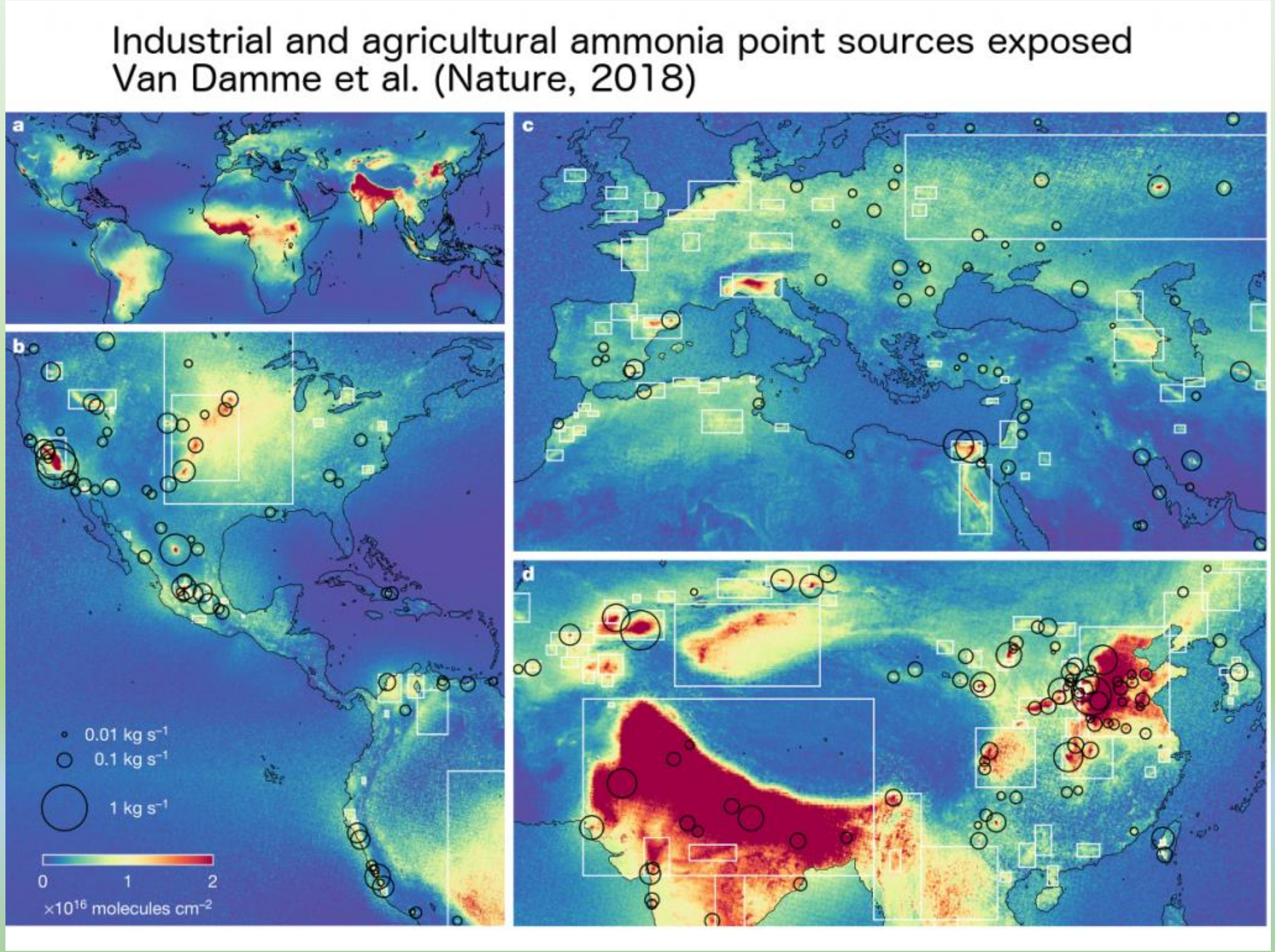
- Extended in space
- Local in time

The issue of NH_3 deposition near hot spots

Remote sensing tools clearly shows large

Global hot spots in India, China and west-Africa

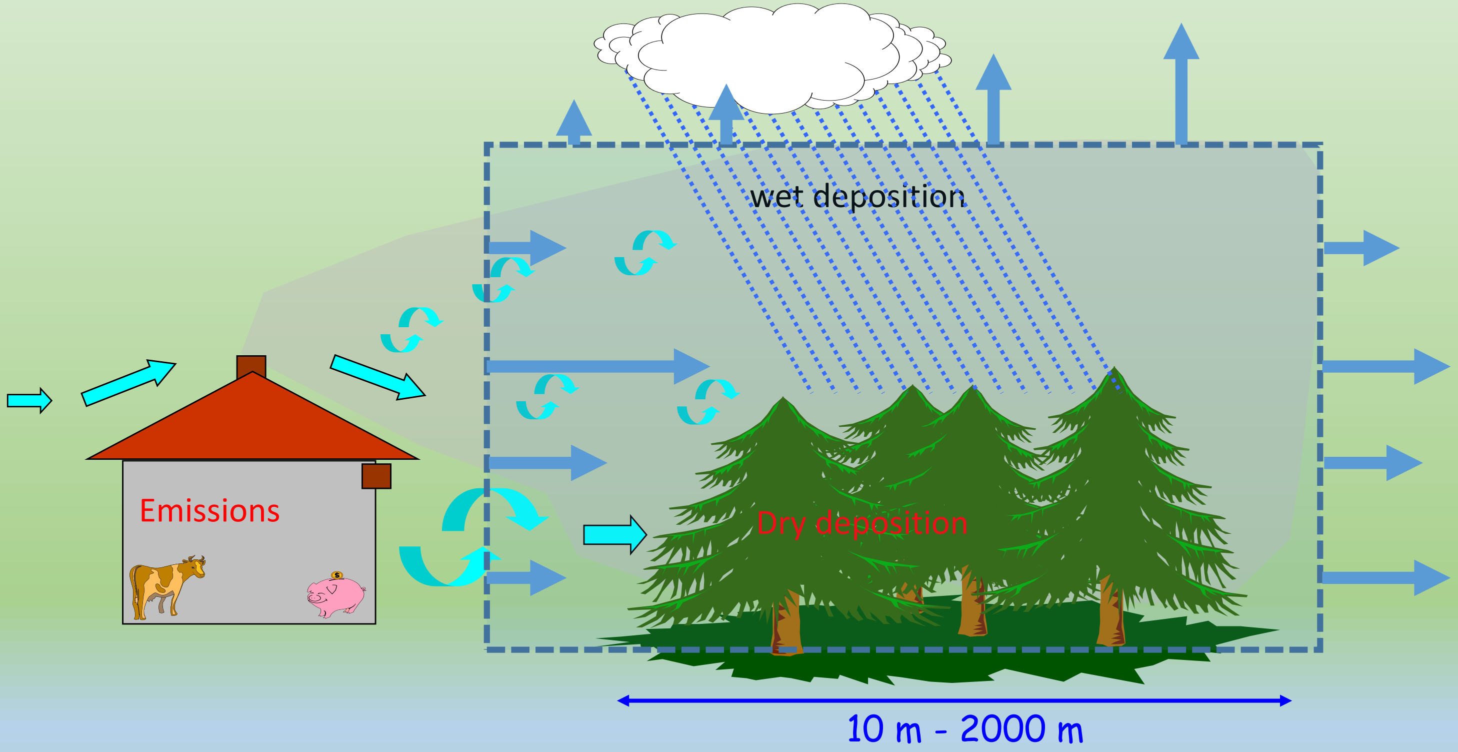
Local hot-spots in America and Europe



Industrial and agricultural ammonia point sources exposed
Van Damme et al. (Nature, 2018)

Challenges of measuring NH_3 deposition near hot spots

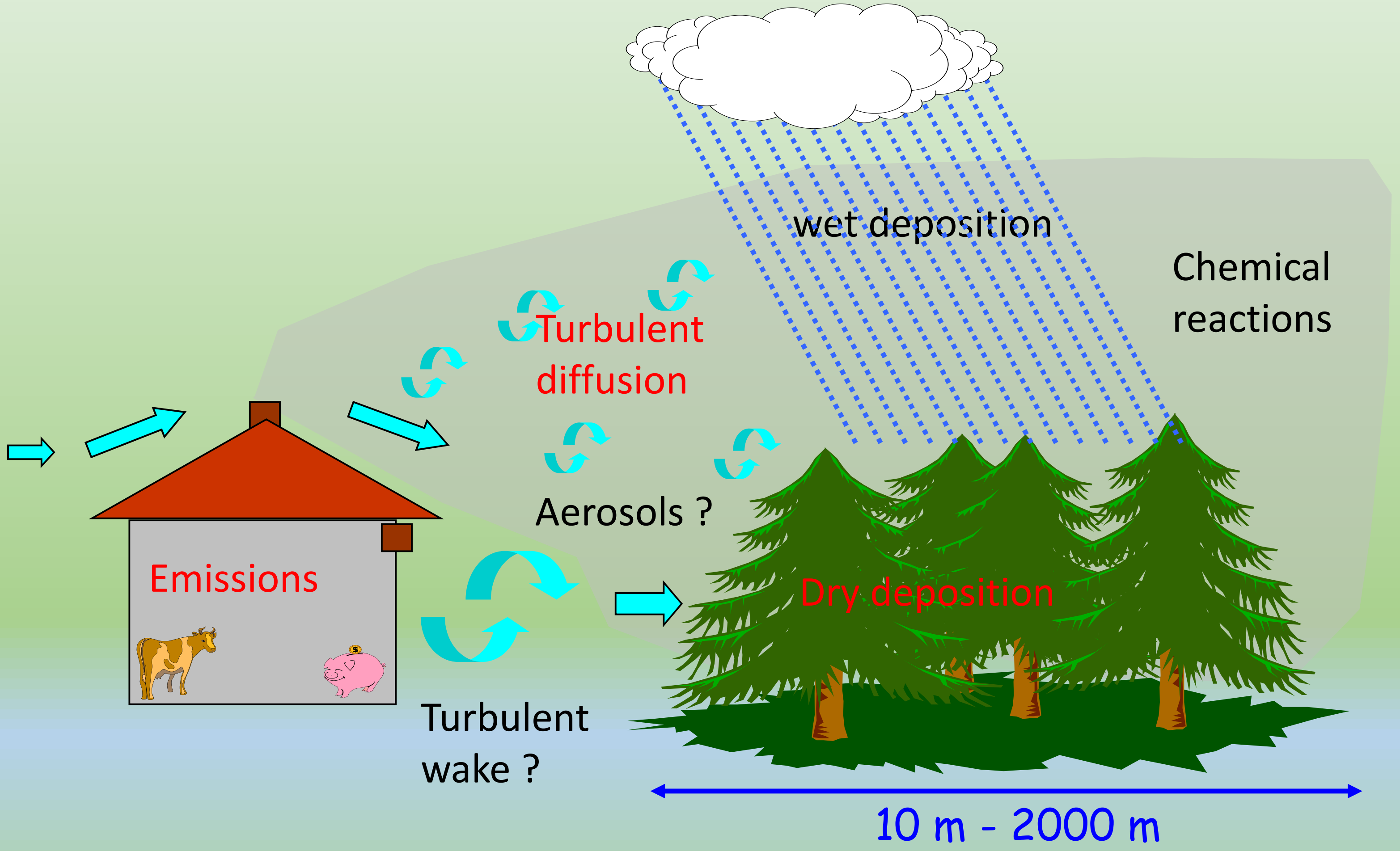
- Direct flux measurement would need to do a mass balance
- This means integrating vertical and horizontal fluxes Ammonia
- Direct surface deposition measurement is not possible because NH_3 flux is an equilibrium process
- Tracer measurement is not easy and require high spatial sampling



⇒ Modelling remains an necessary approach

Challenges of modelling NH_3 deposition near hot spots

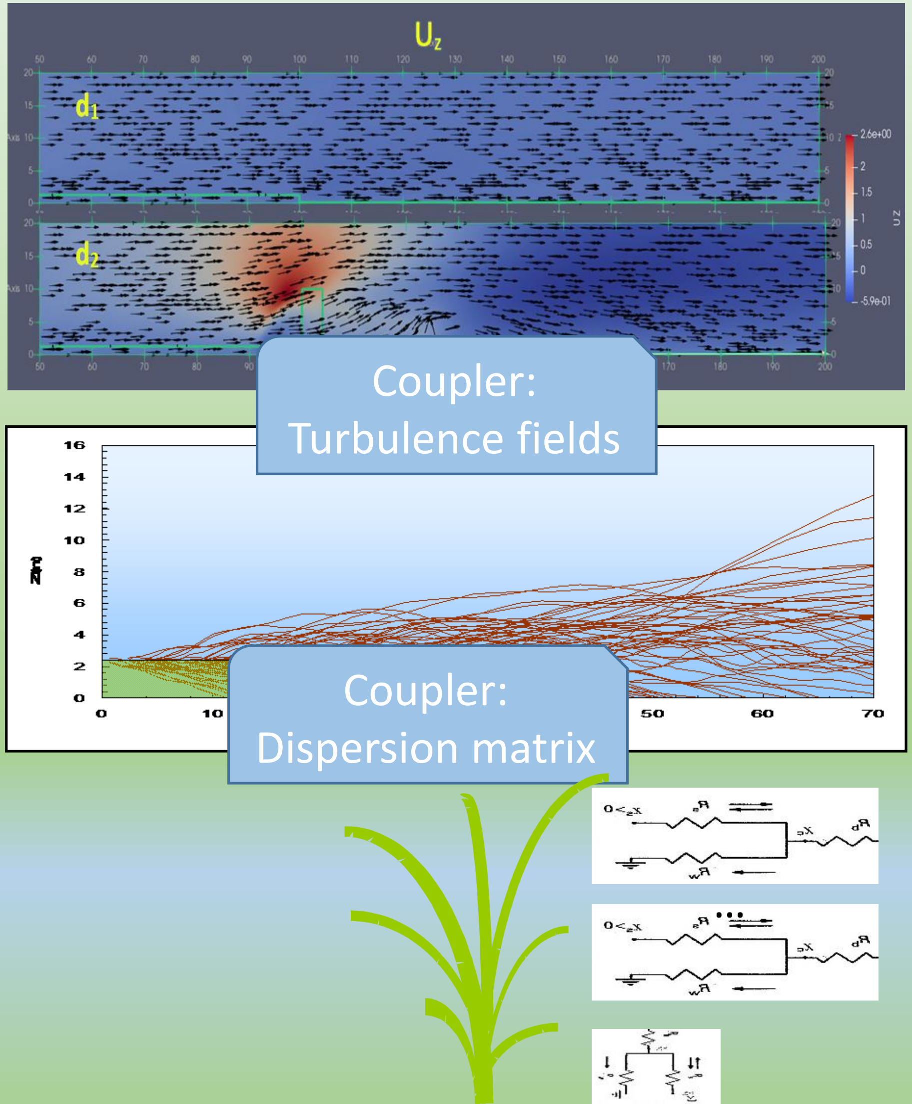
- Model the turbulent flow in a complex situation (k-epsilon or Large Eddy Simulation)
- Account for buildings and transport through the canopy
- Model the deposition to the leaves and ground
- Requires knowledge on surface concentrations and resistances



Ammonia Deposition Near Hot Spots: Processes, Models and Monitoring Methods. Loubet et al. 2009

A model coupling k-epsilon turbulence, Lagrangian Stochastic dispersion and resistance-based deposition

2-dimensional and neutral



Coupler: Turbulence fields

Coupler: Dispersion matrix

OpenFoam k-ε Eulerian turbulence model

- k-epsilon turbulence model
- In-canopy turbulence
- Standard Monin-Obukhov profiles as limits conditions

www.openfoam.com

Lagrangian Stochastic particle dispersion model

- Langevin equations following the particle position

Multi-layer resistance scheme

- for each layer
- Stomatal and cuticular resistance
- Plant and ground compensation point

Loubet et al. 2006. Bealey et al., 2014

The k-epsilon turbulence model and how it is coupled with the Lagrangian Stochastic model

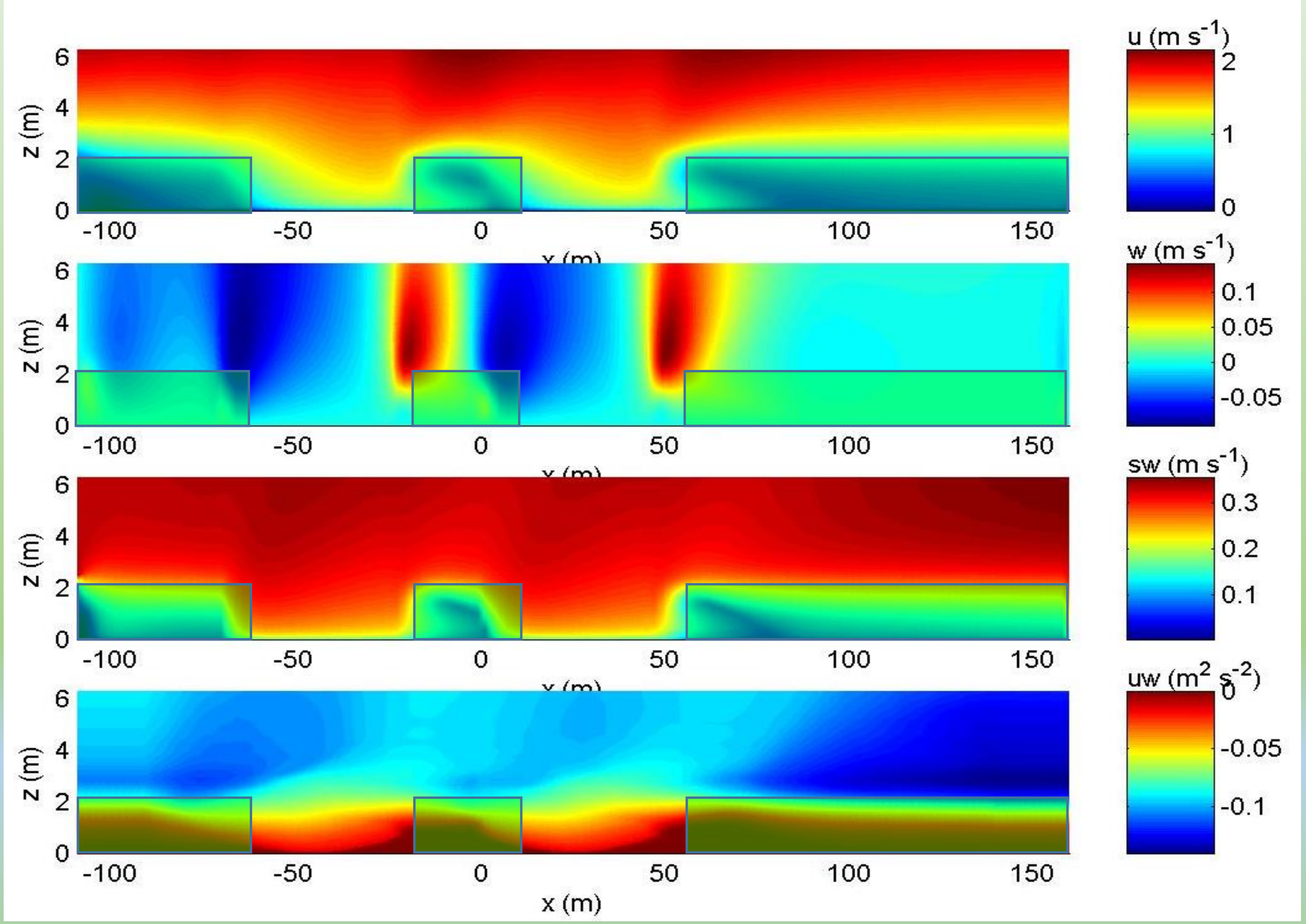
- k-epsilon model provides mean, variance an covariance of wind velocity fields as well as ε (dissipation of turbulent kinetic energy to heat)

Outputs of a k-epsilon model

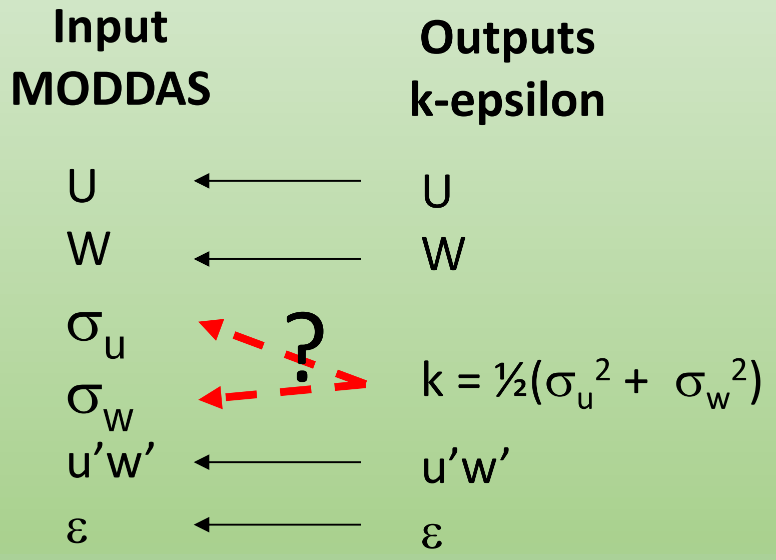
U
W

$k = ½(\sigma_u^2 + \sigma_w^2)$

u’w’
ε



The k-epsilon turbulence model and how it is coupled with the Lagrangian Stochastic model



Input MODDAS	**Outputs k-epsilon**
U	U
W	W
σ_u	
σ_w	$k = ½(\sigma_u^2 + \sigma_w^2)$
u'w'	u'w'
ε	ε

H1. Lagrangian diffusivity K_z^L = Turbulent diffusivity K_z^E

$$K_z^L = \sigma_w^2\, T_L = K_z^E = \frac{C_\mu k^2}{Sc\,\varepsilon}$$

Sc = 0.6

H2. The ratio $\frac{\sigma_u}{\sigma_w}$ is constant (= 1.25)

$$\sigma_u = 0.73(2k)^{0.5}$$
$$\sigma_w = 0.58(2k)^{0.5}$$

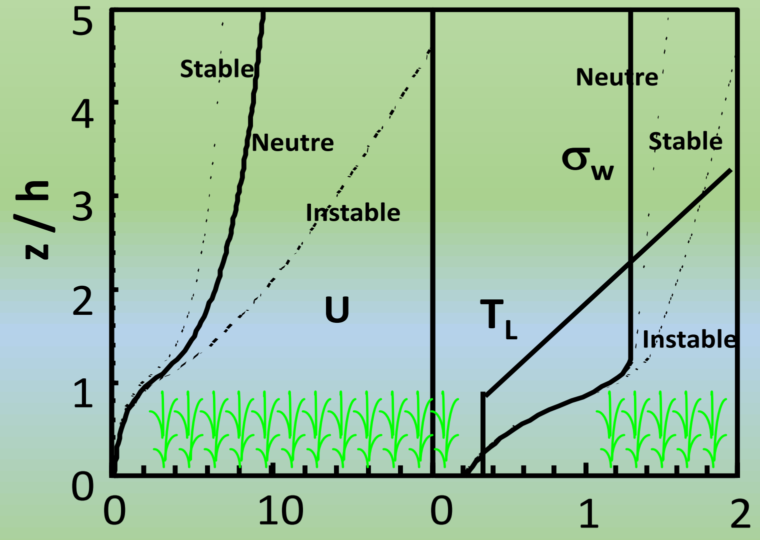
Bealey et al., 2014

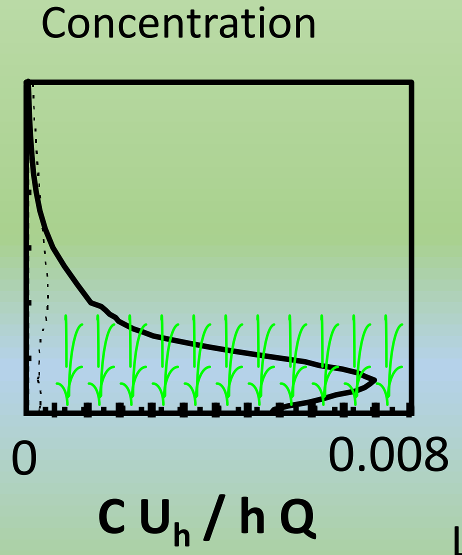
The Lagrangian Stochastic dispersion model

Lagrangian Stochastic model after Thomson (1987)
Random velocity and position
Two dimensional, stationary
Explicit transfer through vegetation
Similar to WindTrax equations (Flesch and Wilson)

Parameters: turbulence *u*, σ_w *u'c'* and Lagrangian time scale, T_L

$$\tau_{Lw} = 2\frac{\sigma_w^2}{3.12\varepsilon}$$



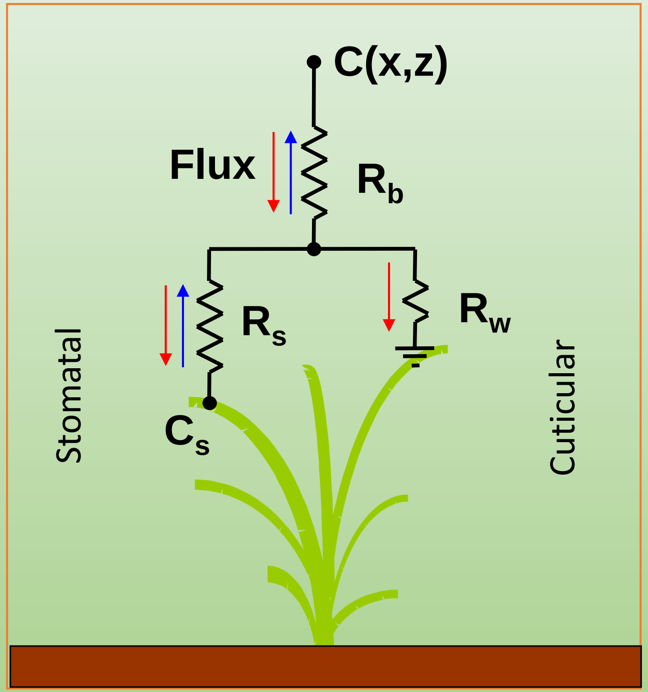


Loubet et al. 2006

Resistance analogy for dry deposition

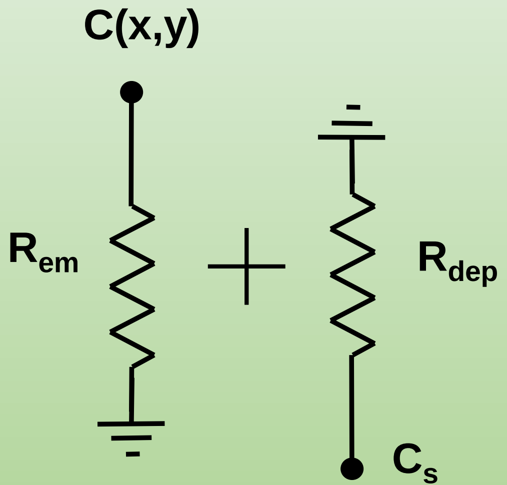
An equivalent scheme is computed with

- an **emission** towards an atmosphere free of ammonia and
- A **deposition** towards a ground that is free of ammonia



C(x,z) : concentration in the canopy
Cs : stomatal compensation point
Rb: leaf boundary layer resistance
Rs : stomatal resistance
Rw : cuticular resistance

See Massad, Nemitz, Sutton. (2010)



$$R_{dep} = R_b + \left(\frac{1}{R_w} + \frac{1}{R_s}\right)^{-1}$$

$$R_{em} = R_b + R_w + R_s\frac{R_w}{R_b}$$

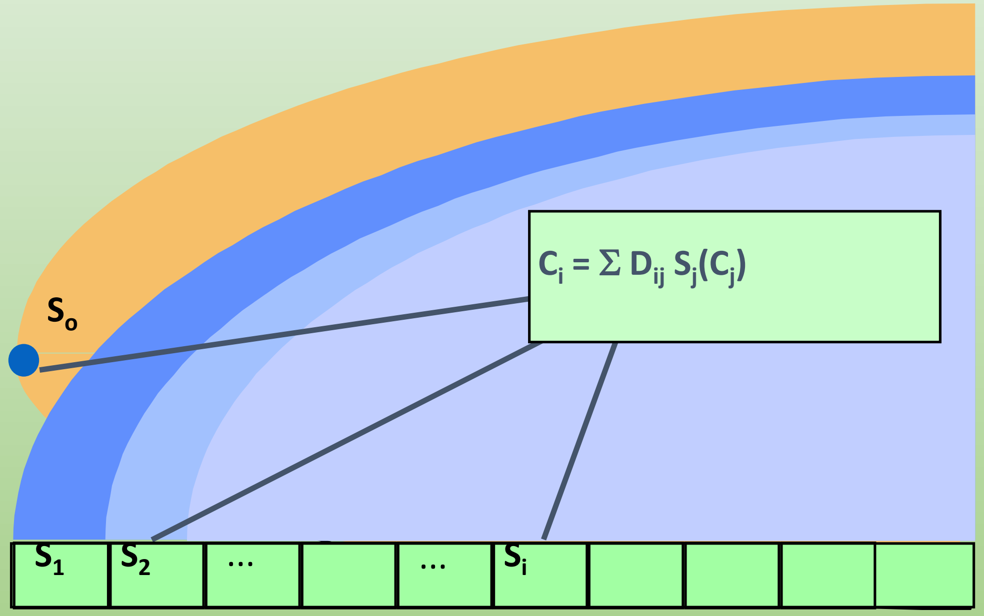
Loubet et al. 2000

Coupling between dispersion and deposition

Coupling is done with the **dispersion matrix** approach:

The dispersion matrix is the **concentration due to each canopy grid cell being a unit source**

The **system is inverted** thanks to the separation of the emission and deposition terms and linearity



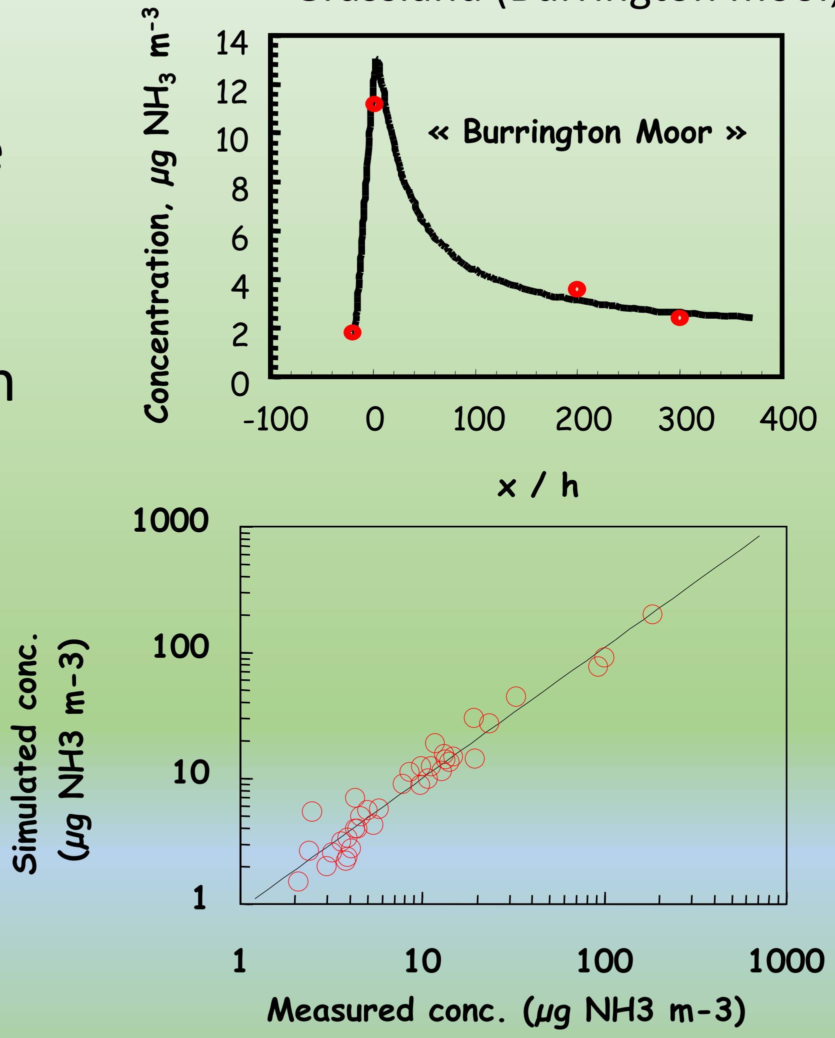
Dispersion matrix approach

Some model “validation”

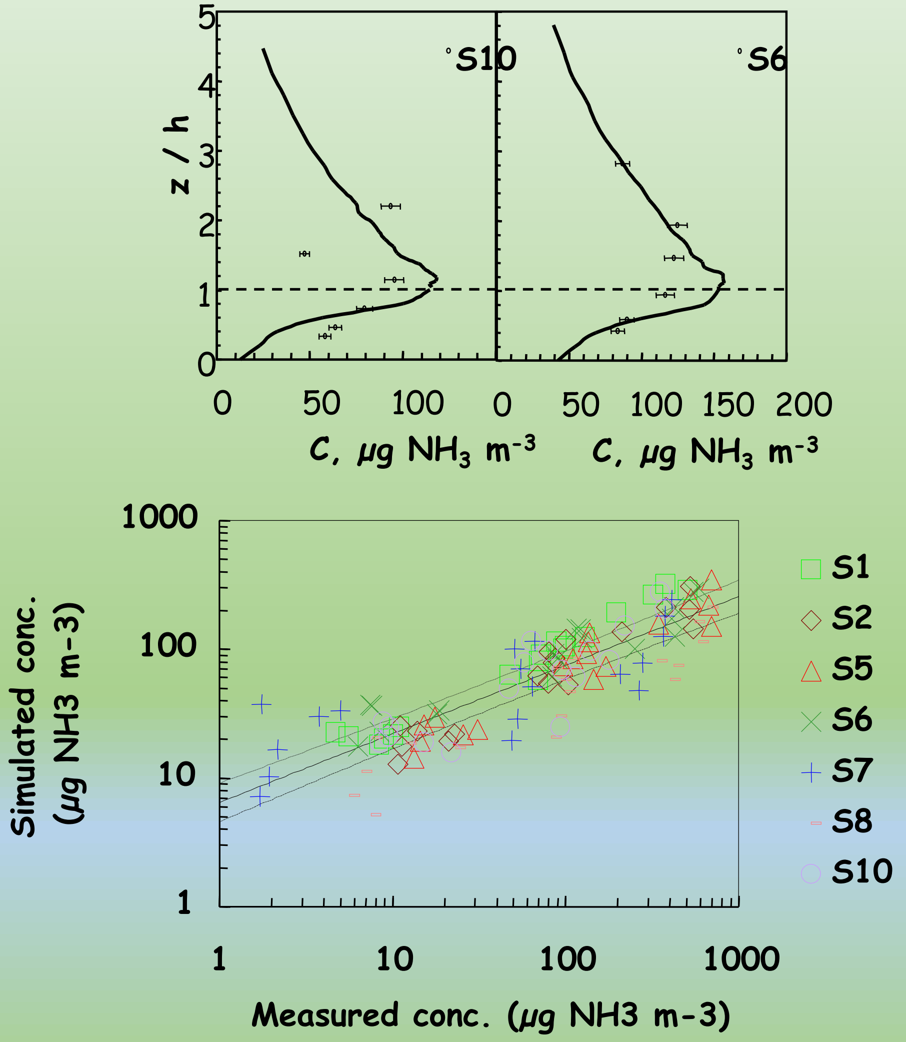
Mainly validation of the dispersion scheme

But impossible to validate the deposition in itself

Grassland (Burrington moor, UK)

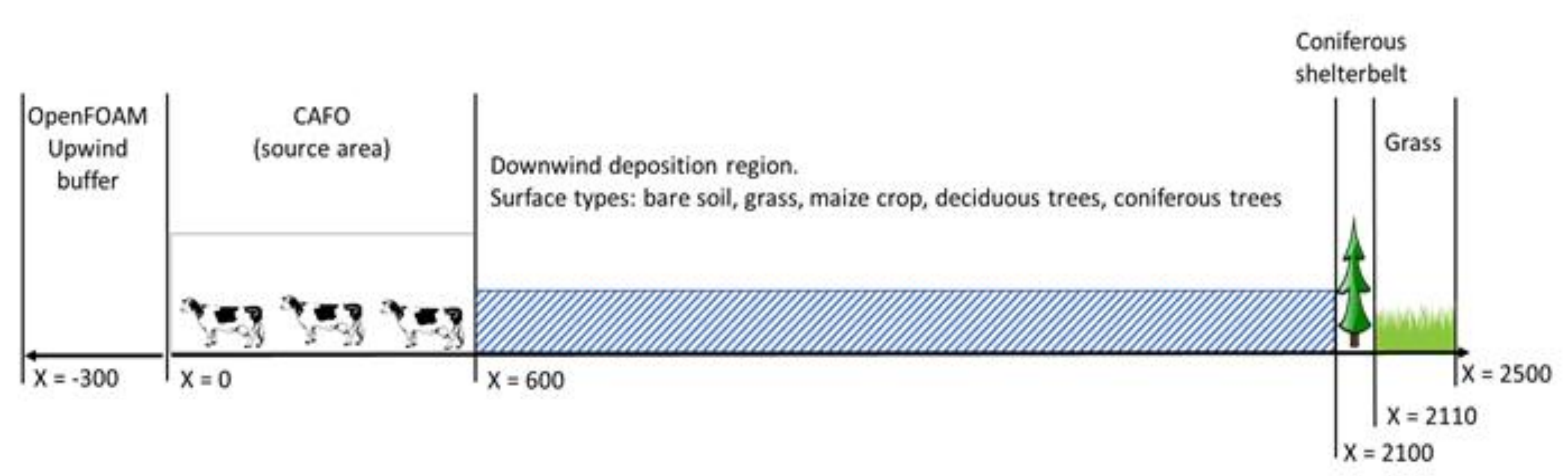


Maize (~Grignon, France)



Application to large feedlots in the USA

	Model Configuration 1
T [degrees C]	8 – 26
RH [%]	70 – 30
U at 15 m	6.8 [m s^{-1}]
Atmospheric Stability	Neutral
Time of day [Local Standard time]	1300
Degrees Latitude	45
Photosynthetically Active Radiation [w m^{-2}]	600
Source Length [m]	600
Source Emission Flux [μg m^{-2} s^{-1}]	100



Emission representative of large US feedlots systems (CAFO)

5 surface types downwind from the feedlot

Lassman et al. in prep.

Application to large feedlots in the USA

Surface concentration is expressed through the emission potential Γ

$$\Gamma = \frac{[NH_4^+]}{[H^+]} = C_s * f(Temperature)$$

Both ground and stomatal emission potential were considered

Massad, Nemitz, Sutton. (2010)

Model parameters

Parameter	Units	Bare Soil	Grass	Maize	Deciduous	Coniferous
H	m	--	0.5	2.5	25.75	19.3
LAI	--	--	2.0	4.5	3.29	6.12
Γ_s	NA	N/A	800	1186	600	1300
Γ_g	NA	360	360	13000	20	20
$R_{w,min}$	$s\ m^{-1}$		30			
$R_{w,\beta}$			2.7			
$R_{s,min}$	$s\ m^{-1}$		60			
$R_{s,\beta}$			7			

Lassman et al. in prep.

Application to large feedlots in the USA

Large effects of trees on wind speed and turbulent kinetic energy

Maize also affects turbulence

Trees create shelter close to the source and to the ground (with less dilution)

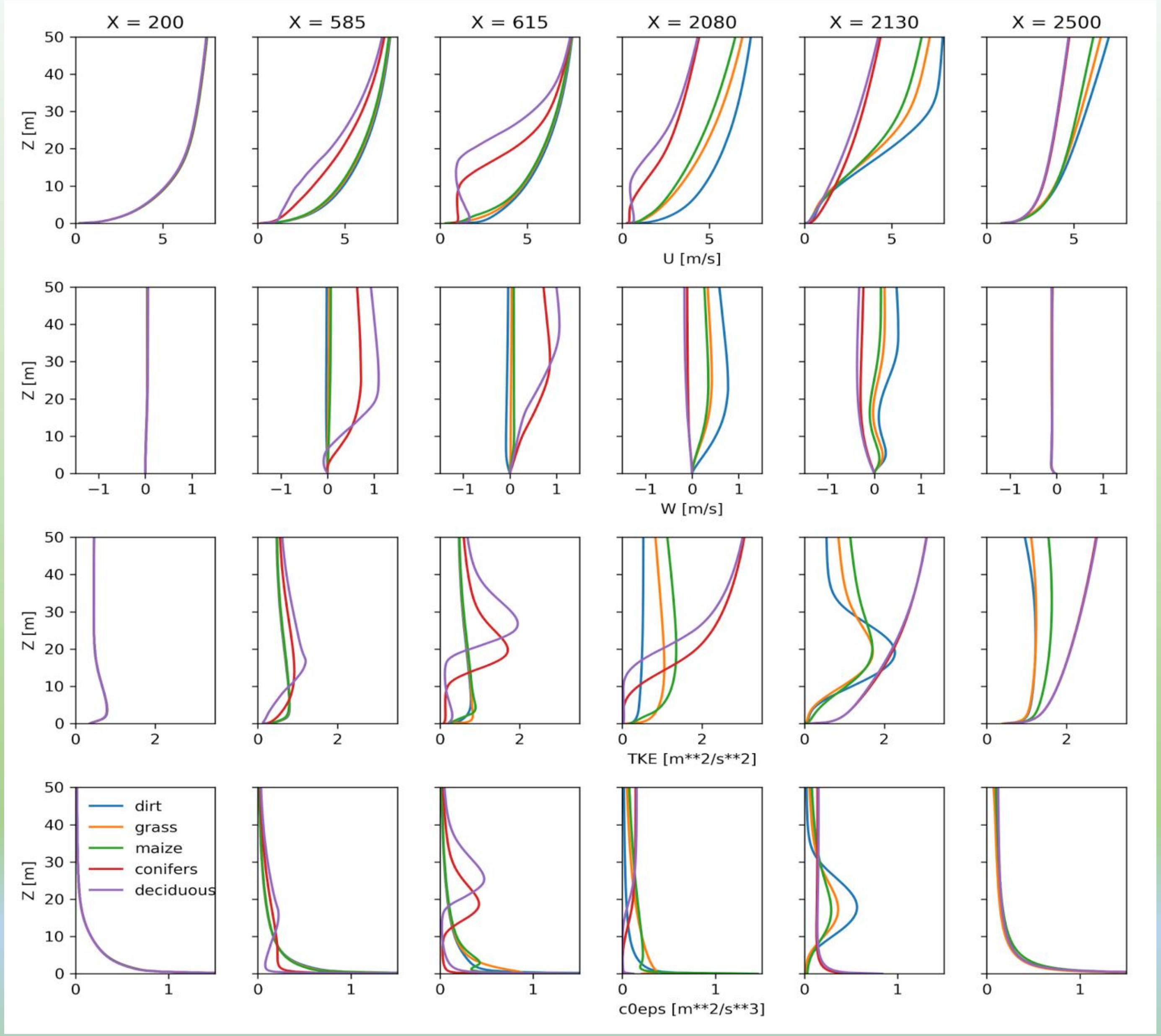


Figure: Vertical profiles of U, W, k, and $C_0\epsilon$ for the simulation Configuration

Lassman et al. in prep.

Application to large feedlots in the USA

Concentration in the feedlot are up to 1 mg NH_3 m^{-3} up to 20 m height

Maize diminishes substantially the NH_3 concentration at the surface but increases it above 20 m height

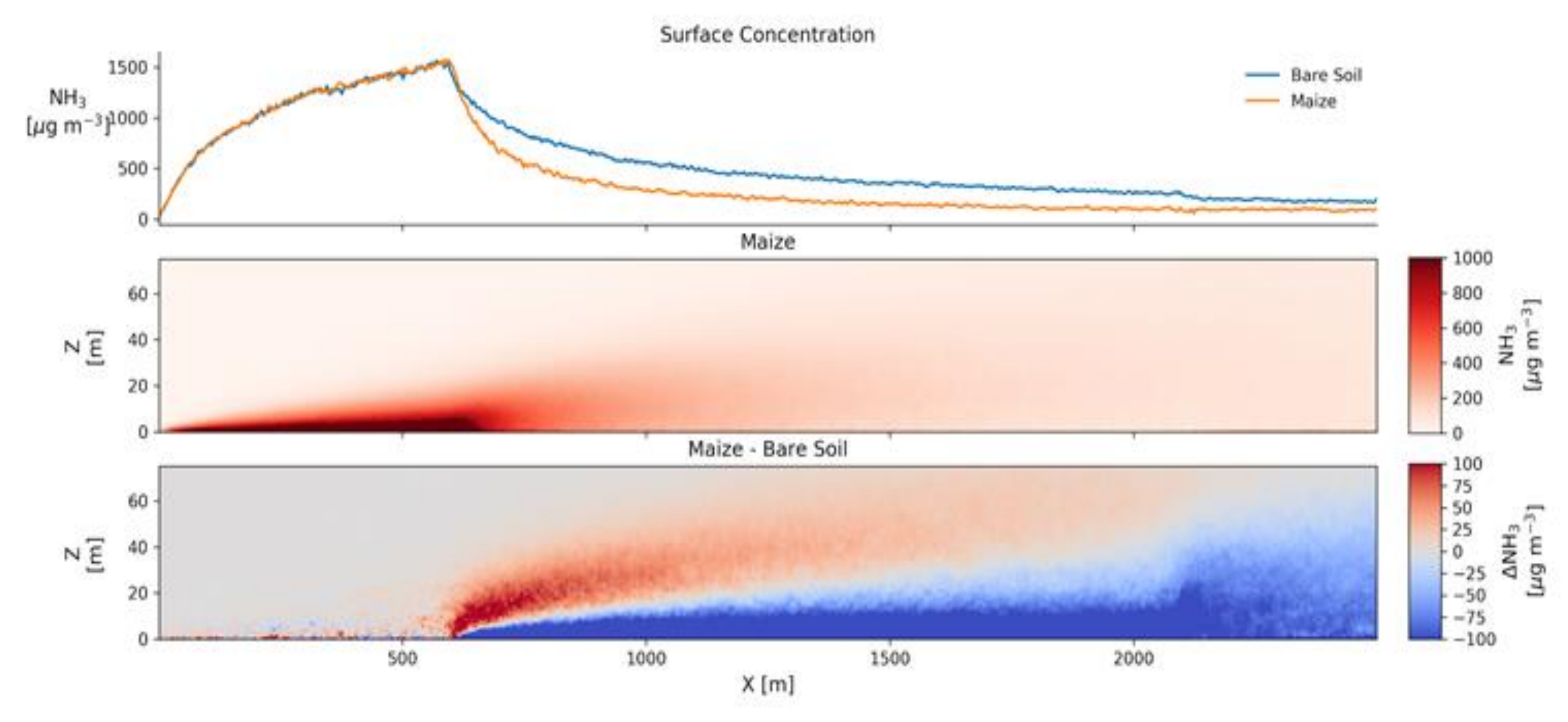


Figure: (a) surface concentration, (b) concentrations in the atmosphere, (c) concentration difference between maize and bare soil simulation cases.

Lassman et al. in prep.

Application to large feedlots in the USA

Deposition in the first ~200 m downwind from the feedlot is key

Trees show up to 50% recapture efficiency

Maize could also substantially recapture ammonia (30% recapture)

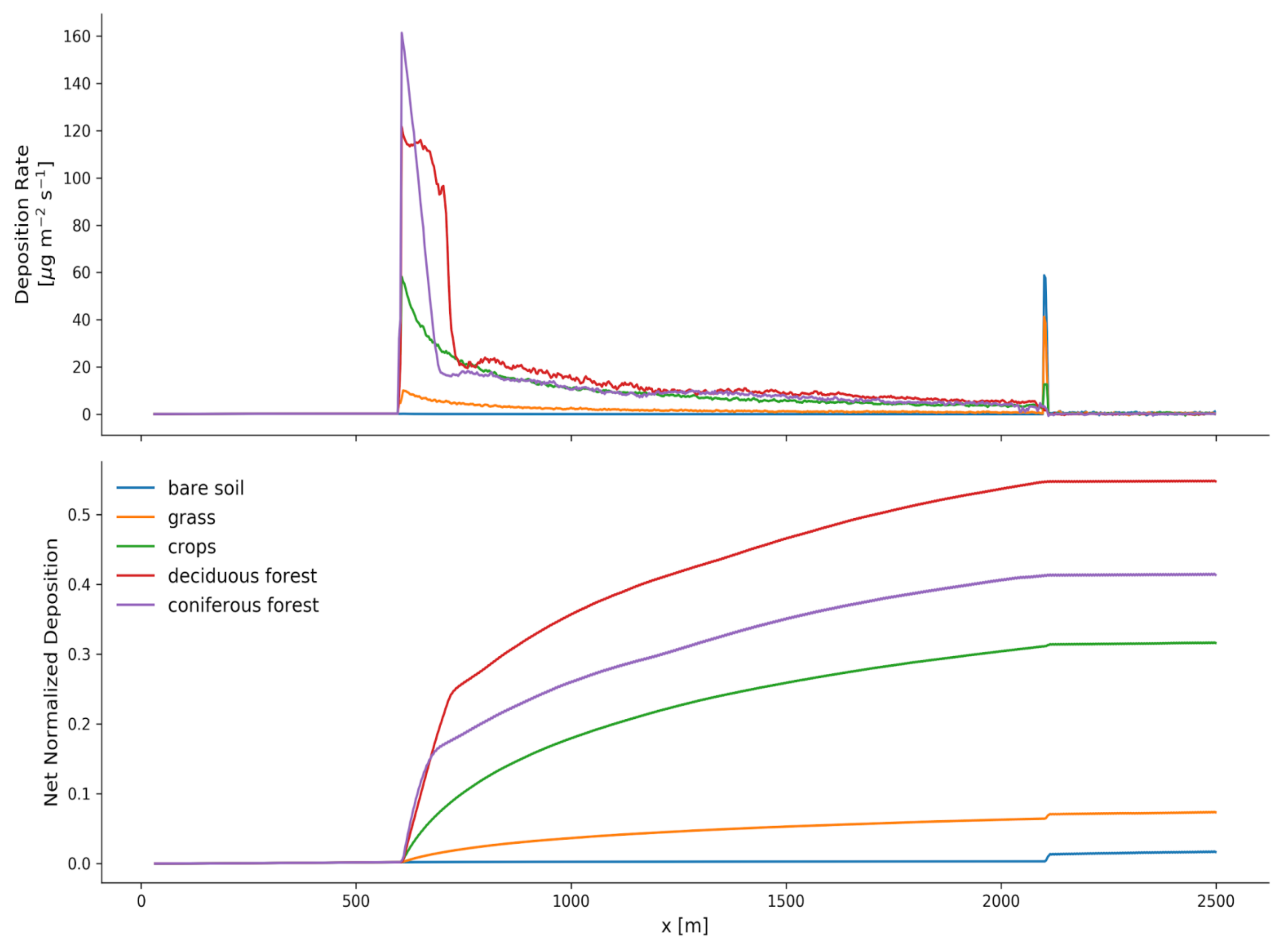


Figure: Ammonia deposition depending on land-use type

Lassman et al. in prep.

Application to large feedlots in the USA

Deposition highly dependent on the ammonia compensation point of the downwind vegetation …

… but also on the temperature and humidity status of this vegetation

The benefit of recapture could be lost with highly fertilised crops in hot and dry conditions

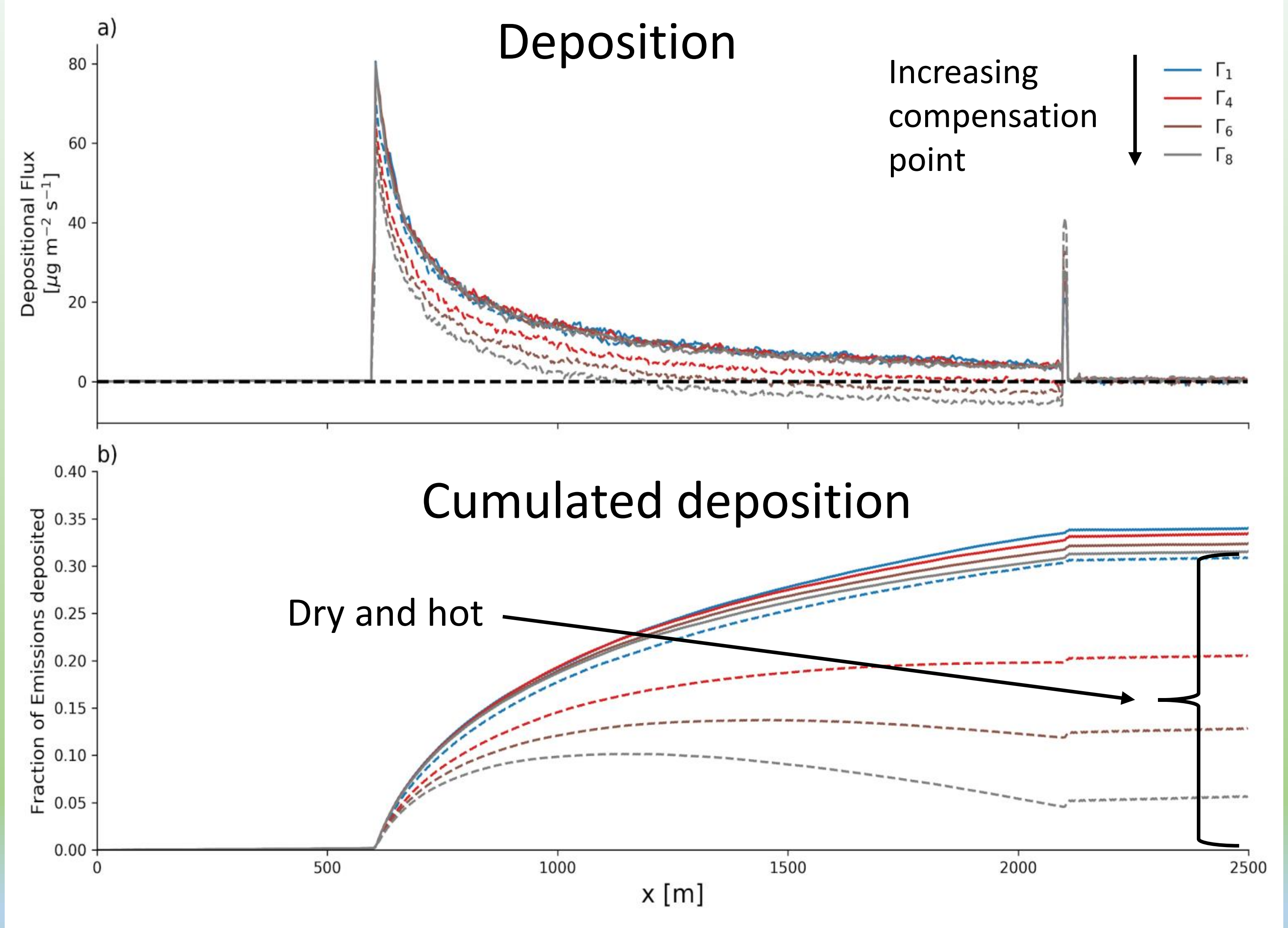


Figure: Ammonia deposition sensitivity to surface concentration (expressed as emission potential Γ) and surface temperature. Γ_1 = 1200, Γ_8 = 33000.

Lassman et al. in prep.

Application to large feedlots in the USA

Same as previous slide but with another way to represent it.

Temperature is the main driver with large emission potential

RH is the driver with low emission potential

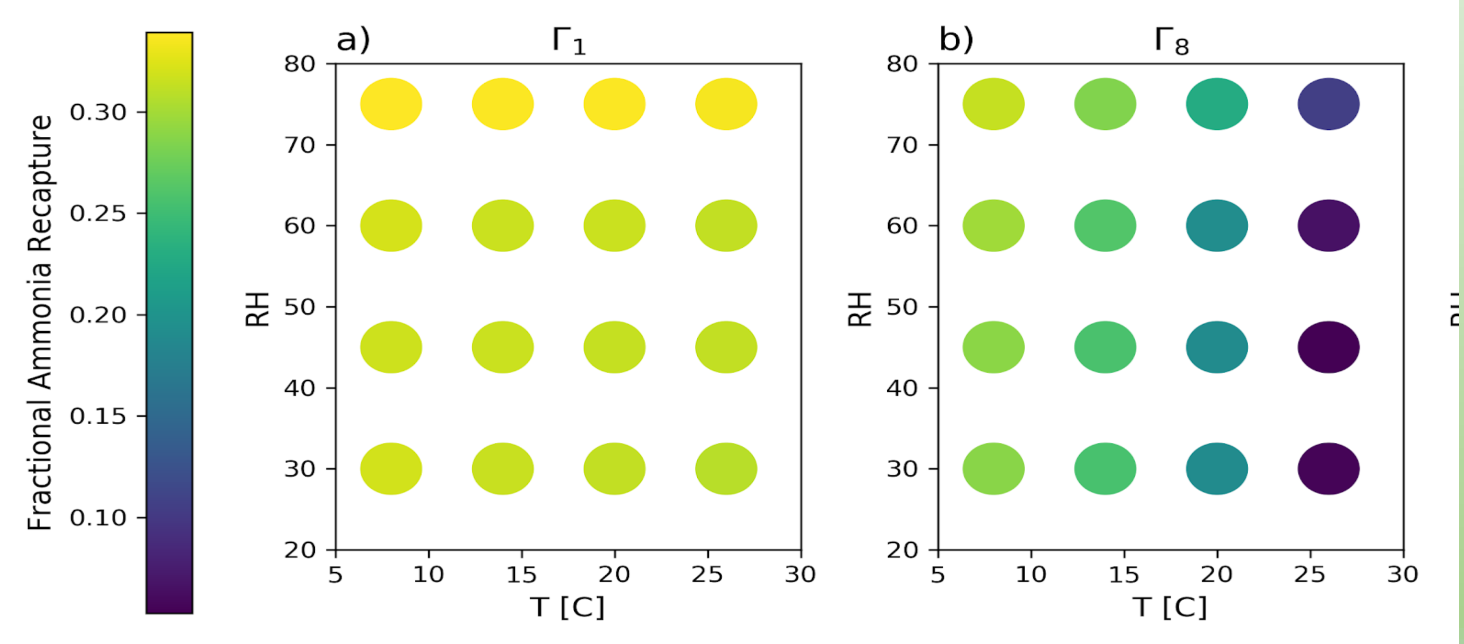


Figure: Impact of T, RH and the emission potential Γ on the ammonia recapture fraction. $\Gamma_1 = 1200$, $\Gamma_8 = 33000$.

Lassman et al. in prep.

Application to a tree recapture belt in the UK

Similar simulations on three scenarios : Housing, Lagoon and understory.

Configuration with a tree belt and a “backstop” to maximise the filter effect

Simulation over a year with monthly mean parameters

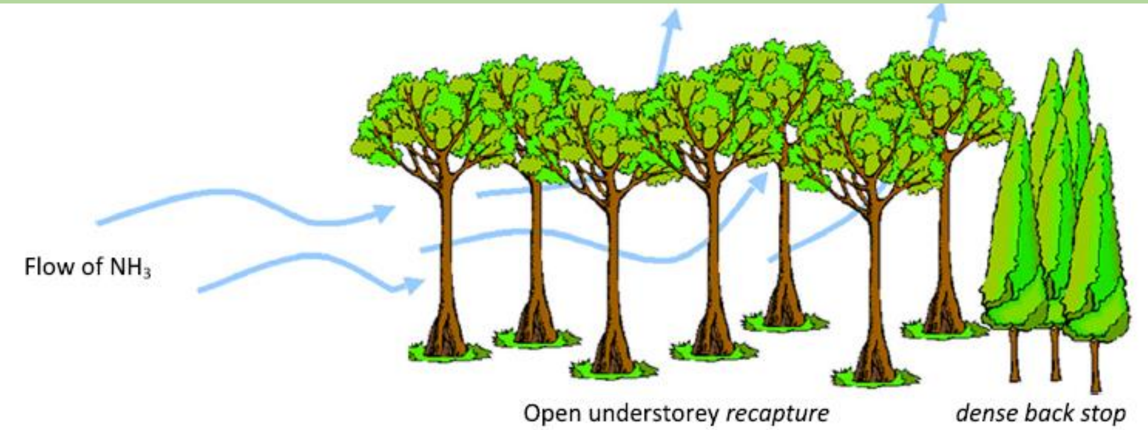


Figure 1. Schematic diagram of a tree belt design to maximize recapture of ammonia. From Theobald *et al* (2003).

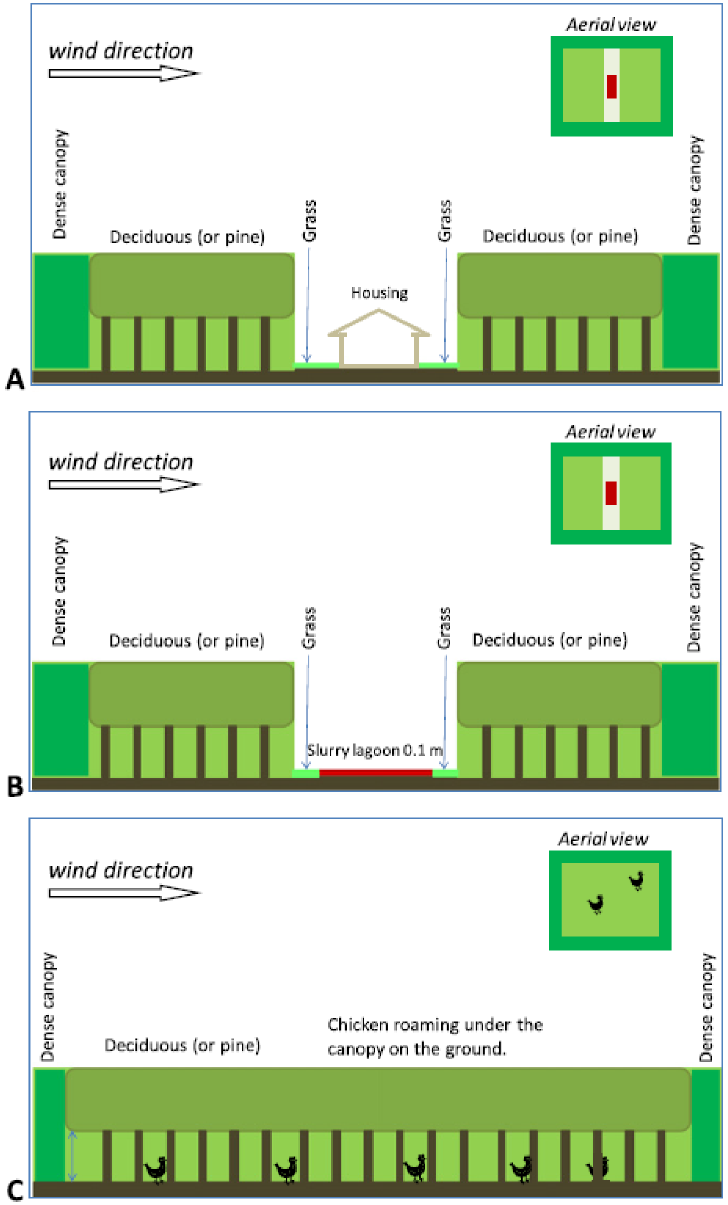
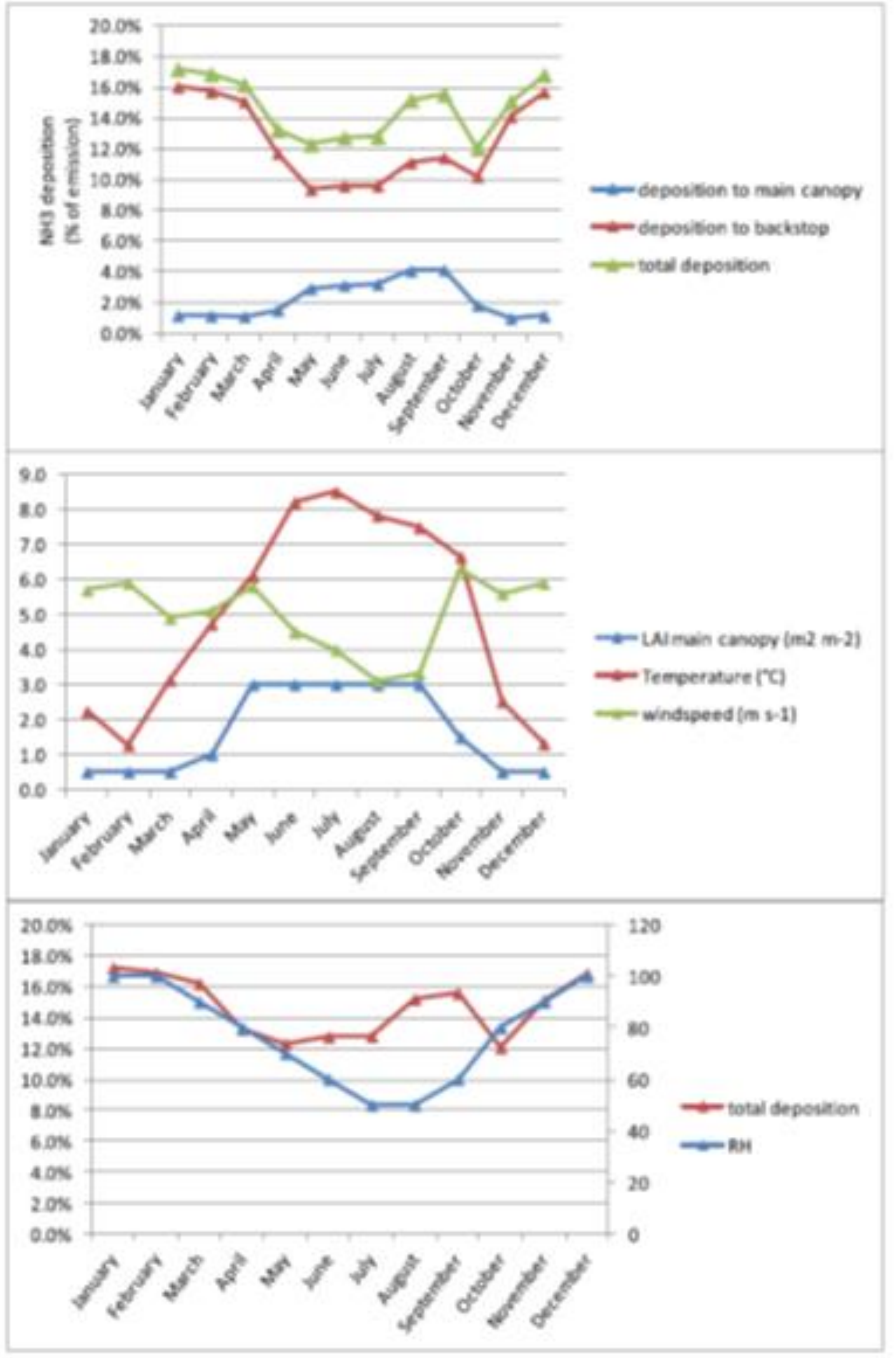


Figure 4. Visualization of example source types for tree belts upwind and downwind: (A) Housing source type. (B) Lagoon source type (red line), a variant of the housing scenario and (C) under-storey source scenario with free-ranging chickens. The 2D aerial view (top right) shows the scheme from above.

Bealey et al. 2014

Application to a tree recapture belt in the UK



Deposition can reach 50% in case of understorey

Rather around 20% maximum for the other situations

Similarly as in Lassman et al., we find a large dependency on climatic conditions (humidity) …

… but also on tree physiology (leaf area index)

Bealey et al. 2014

Conclusions

- Modelling dry deposition of NH3 downwind from hot spots is of key interest to decrease emissions and protect local biodiversity
- A model coupling a k-epsilon turbulence model to a Lagrangian-Stochastic and resistance exchange model have proven to be an efficient way to address this issue
- Ammonia recapture rates by tree or crop-belts range from 5% to 50% and are highly dependent on the surface emission potential Γ, humidity and temperature
- Large ammonia deposition rates in tree or crop-belts would induce an increase of the surface emission potential which may limit the interest in such systems over time
- A remaining challenge is to understand and model these feedback effects which can act on surface ammonium concentration and or pH

Thanks for your attention

references

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The Lagrangian Stochastic model for pesticides drift

Lagrangian Stochastic model of « **fluid parcels** »

$$\begin{cases} d\boldsymbol{u} = \boldsymbol{a}(\boldsymbol{u}, \boldsymbol{v_p}, \boldsymbol{x}_p, t)\mathrm{dt} + \mathbf{b}(\boldsymbol{u}, \boldsymbol{v_p}, \boldsymbol{x}_p, t)\, d\boldsymbol{\xi} \\ d\boldsymbol{x_p} = \boldsymbol{u}dt \end{cases}$$

Equation of motion of the **droplet**

$$d\boldsymbol{v_p} = \frac{(\boldsymbol{u}-\boldsymbol{v_p})}{\tau_p}\, dt - m_p \boldsymbol{g}\, dt$$

Adaptation for pesticides

- The inertia of droplets was neglected in the transport
- Inertia accounted for in the initial velocity only
- Droplet evaporation added
- Impaction adapted to high velocities (Mirzaee et al. 2019)

Initial velocity inertia $\boldsymbol{v_p^*} = \boldsymbol{v_0}\, exp^{(-t/\tau_p)}$

Droplet displacement $d\boldsymbol{x_p} = (\boldsymbol{u} + \boldsymbol{v}_p^* - v_s)dt$

Droplet evaporation $d_\mathrm{p} = d_\mathrm{p}^0 * \left(1 - \frac{t}{\tau_e}\right)^{1/2}$

$\boldsymbol{u}$ fluid velocity	(m s^{-1})
$\boldsymbol{v_p}$ particle velocity	(m s^{-1})
$\boldsymbol{x}_p$ particle position	(m)
$\boldsymbol{d_p}$ particle diameter	(m)
ρ_p particule density	(kg m^{-3})
g gravity acceleration	(9.81 m s^{-2})
τ_p particle inertial time	(s)
τ_e evaporation time	(s)
v_s particle settling speed	(m s^{-1})
μ kinematic viscosity	(m^2 s^{-1})
$d\boldsymbol{\xi}$ Wiener increment	($s^{1/2}$)

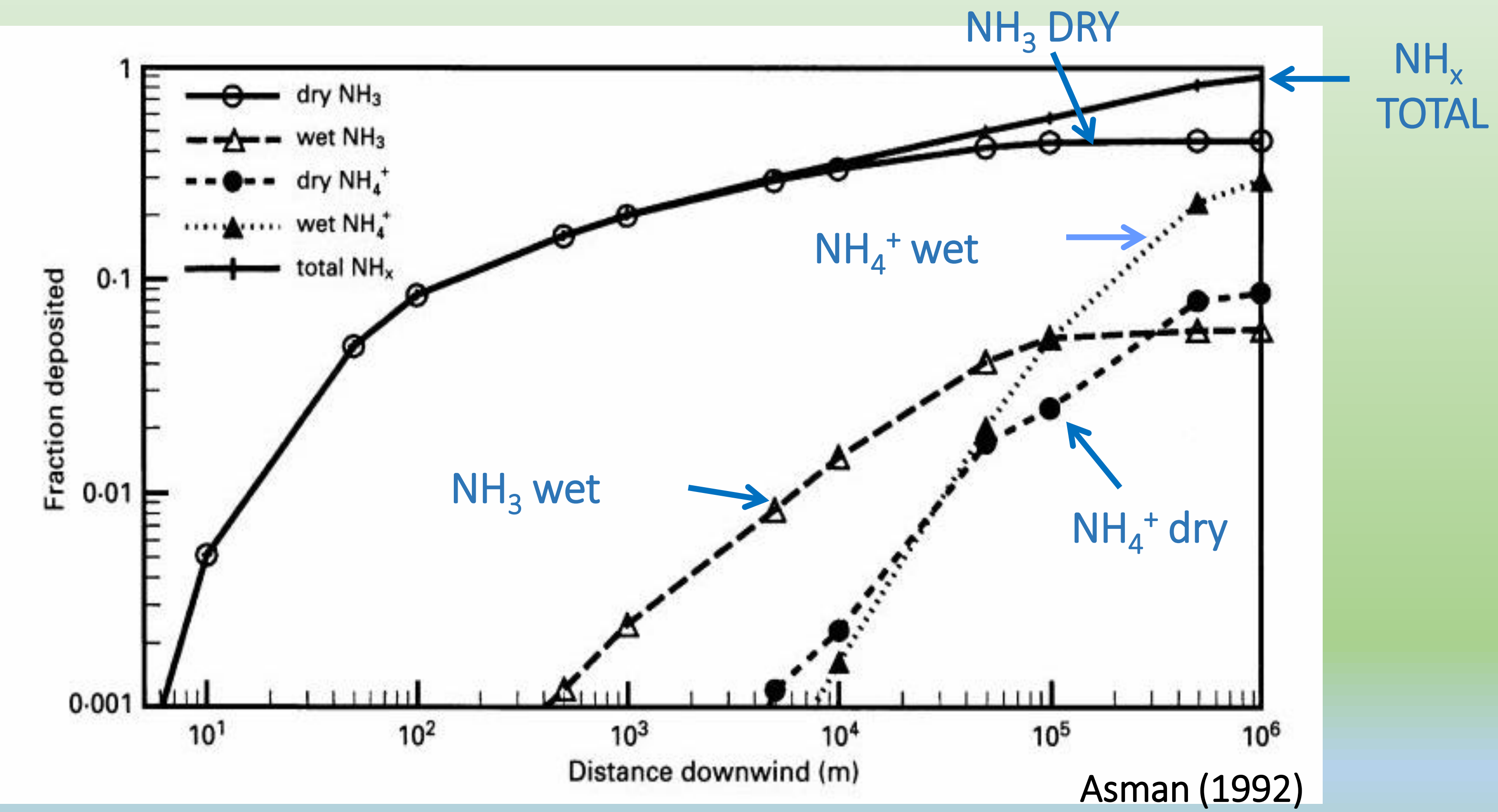
$$v_s = \frac{1}{18}\,\frac{d_p^2\ g\ \rho_p}{\mu}$$

$$\tau_p = \frac{v_s}{g}$$

Djouhri et al. (2023) in press

Challenges of modelling NH_3 deposition near hot spots

- Wet deposition and chemistry transformation could in theory be neglected within a few kilometres



Asman (1992)