The Atmospheric Chemistry and Canopy Exchange Simulation System for Ammonia (ACCESS-NH3): Formulation and Application to a Corn Canopy

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Background

- Agricultural sources (e.g., from waste products of domesticated livestock and fertilizer volatilization) account for nearly 90% of ammonia (NH_3) emissions in the U. S. (Xing et al., 2013).
- Through its reactions with sulfuric and nitric acids, NH_3 contributes to the formation of fine aerosol particles, elevated concentrations of which have been linked to various human health impacts (Pope and Dockery, 2006).
- Removal of NH_3 or fine particle ammonium (NH_4^+) from the atmosphere back to the Earth's surface may have deleterious effects on sensitive terrestrial or aquatic ecosystems (Greaver et al., 2012).
- The bi-directional nature of NH_3 exchange between the atmosphere and biosphere makes modeling difficult for 3-D atmospheric chemistry and air quality models.
- Ammonia interactions with vegetative canopies, where plants can act as either sources or sinks, remain a source of uncertainty in bi-directional exchange models.

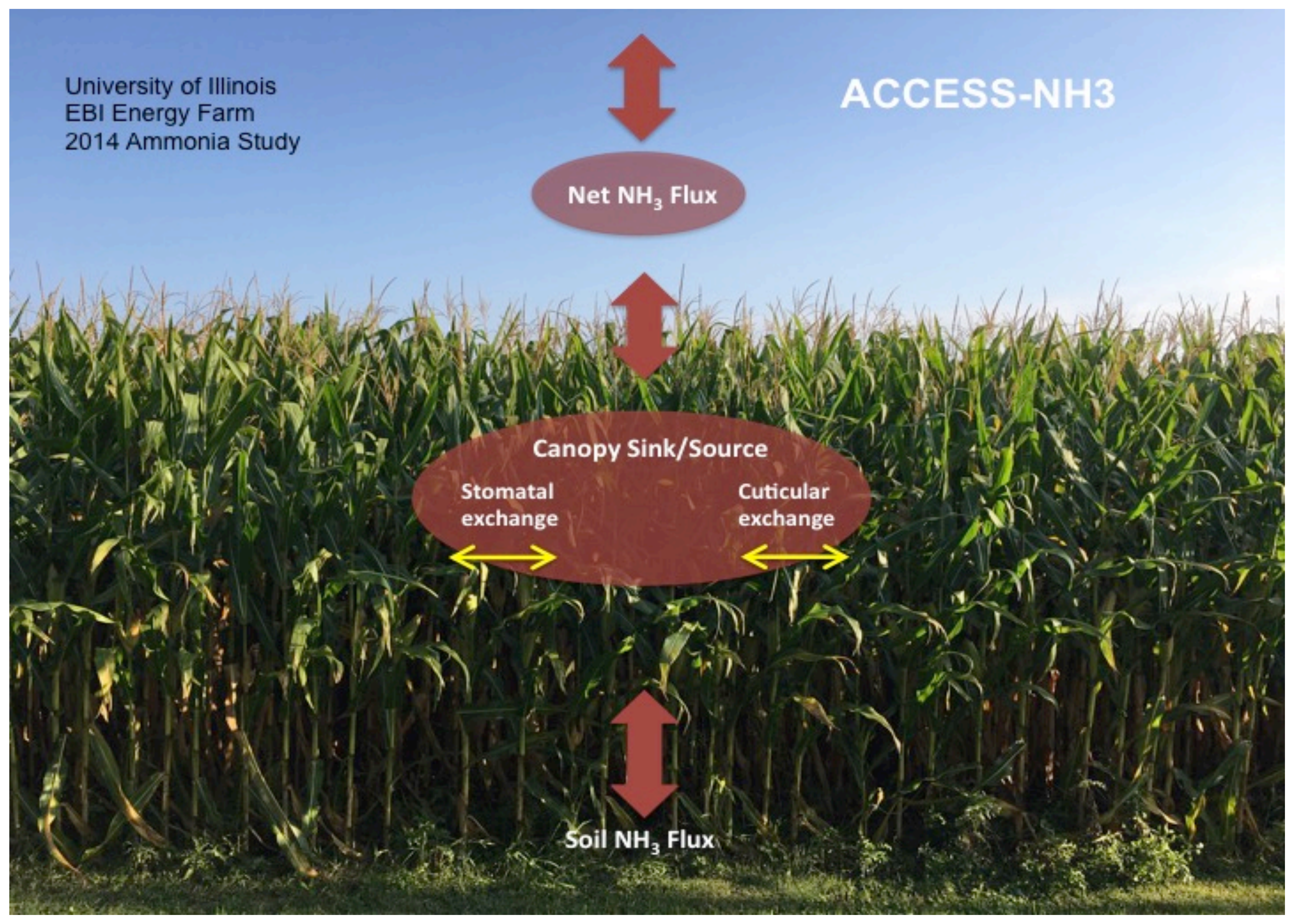

Figure 1. NH_3 bi-directional exchange with a vegetative canopy is an important consideration in modeling. Under what environmental conditions does the canopy act as a source or sink for ammonia?

Model Formulation

The Atmospheric Chemistry and Canopy Exchange Simulation System (ACCESS, Saylor (2013)) is a 1-D column model for simulating emissions, vertical transport, atmospheric chemistry and deposition of trace chemical species within and above vegetative canopies. ACCESS-NH3 is a separate NH_3-specific modeling system for simulating the vertical distribution and fluxes of NH_3 throughout the soil-plant-atmosphere continuum. Its purpose is to improve our understanding of the interactions between atmospheric NH_3 and plant canopies and provide insight on the environmental conditions under which the canopy may act as either a source or sink for NH_3.

The governing equation and initial and boundary conditions for ACCESS-NH3 are given as

$$\frac{\partial \chi(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(\rho(z,t)K_v(z,t)\frac{\partial \chi(z,t)/\rho(z,t)}{\partial z}\right) - v_c(z,t)\left(\chi(z,t)-\chi_c(z,t)\right)\cdot LAD(z) \quad (1)$$

with initial condition

$$\chi(z,t) = \chi_0(z) \qquad @\ t=0 \quad (2)$$

and boundary conditions

$$-\rho(0,t)K_v(0,t)\frac{\partial \chi(0,t)/\rho(0,t)}{\partial z} = -v_s(t)\left(\chi(0,t)-\chi_g(t)\right) \qquad @\ z=0 \quad (3)$$

$$\chi(z>H,t) = \chi_a(t) \qquad @\ z=H \quad (4)$$

The model domain extends from the soil surface up through the plant canopy to a height H where the NH_3 concentration is measured above the canopy. The domain is discretized into equally-spaced levels depending on the height of the canopy and the total domain height. At each level in the canopy, exchange of NH_3 is parameterized with a resistance analogy approach, with details as illustrated in Figure 2. If an effective canopy compensation point at each level n is defined as χ_c, then the component fluxes at each level can be defined as

Total canopy flux at z:
$$F_c(z,t) = -\frac{\chi(z,t)-\chi_c(z,t)}{r_b(z,t)} \quad (5)$$

Stomatal flux at z:
$$F_s(z,t) = -\frac{\chi_c(z,t)-\chi_s(z,t)}{r_s(z,t)} \quad (6)$$

Cuticular flux at z:
$$F_w(z,t) = -\frac{\chi_c(z,t)}{r_w(z,t)} \quad (7)$$

The total canopy flux is the sum of the stomatal and cuticular fluxes,

$$F_c(z,t) = F_s(z,t) + F_w(z,t). \quad (8)$$

The effective canopy compensation point is then determined by combining Eqs. (5)-(8) and solving for χ_c to get (dropping the (z,t) dependence notation)

$$\chi_c = \frac{r_s r_w \chi + r_b r_w \chi_s}{r_s r_w + r_b r_w + r_b r_w}. \quad (9)$$

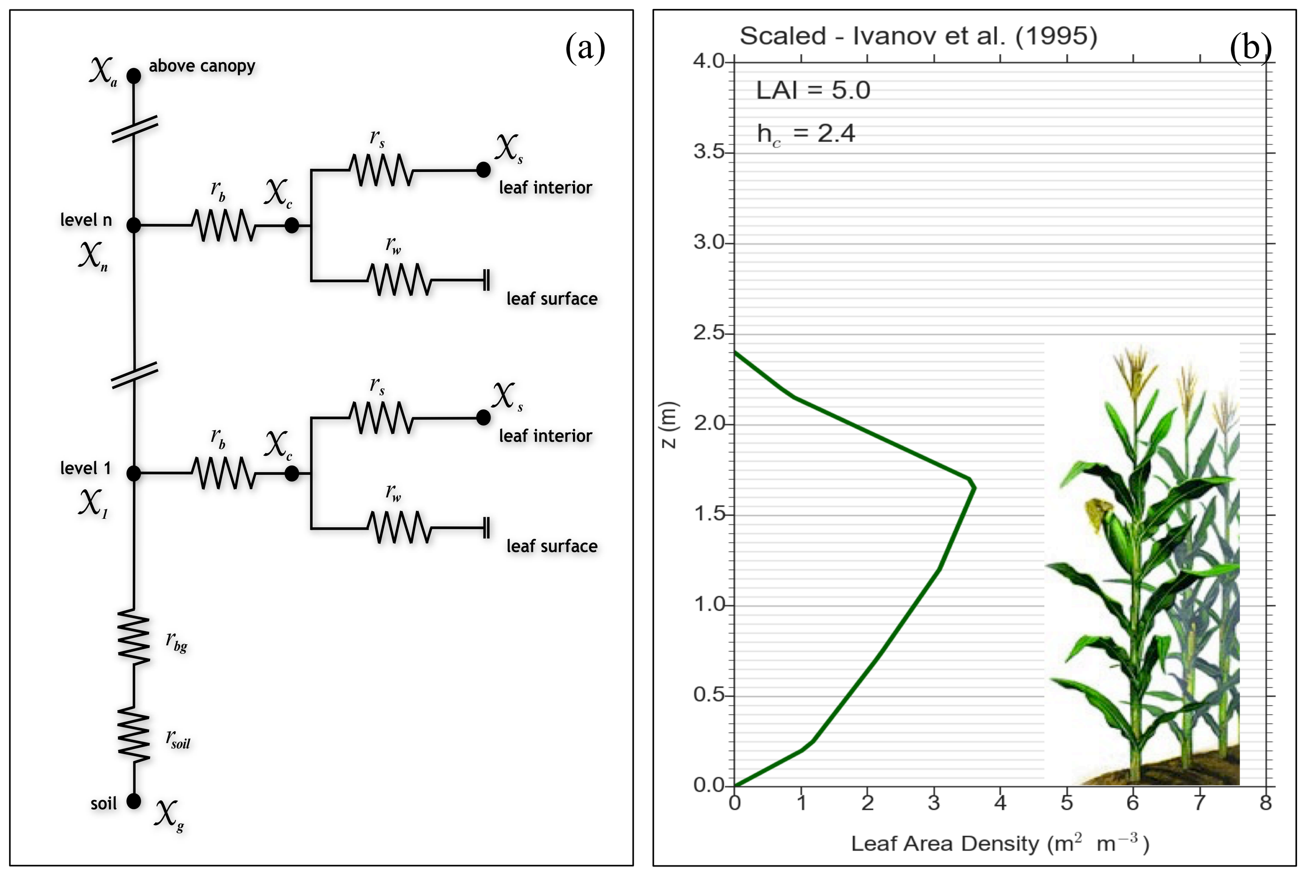

Figure 2.(a) Resistance analogy schematic for NH_3 fluxes as parameterized by ACCESS-NH3; (b) Leaf area density profile used for simulations of June 28-29, scaled from maize canopy measurements of Ivanov et al. (1995).

Simulation Methodology

During the growing season of 2014, measurements of NH_3 concentrations and fluxes, along with extensive meteorological, environmental, and physical crop variables were made above a corn canopy at the University of Illinois at Urbana-Champaign Energy Biosciences Institute Energy Farm in Urbana, IL (Nelson et al., 2017). From these measurements, inputs of above canopy NH_3 concentration, air temperature and humidity, soil temperature and moisture, solar radiation, PPFD, and mean wind speed were used to drive ACCESS-NH3 simulations. Currently, five periods during the 2014 growing period have been simulated: (i) May 31 – June 1; (ii) June 6-7; (iii) June 13-15; (iv) June 21-23; and, (v) June 28-July1. Soil and stomatal emission potentials were estimated based on the work of Lichiheb et al. (in preparation): Γ_{soil}= 10000, Γ_{st} = 500. Preliminary simulation results for June 28-July 1 are presented in Figures 3 and 4. Simulation analyses will continue, including comparison of modeled fluxes to measurements and comparison of ACCESS-NH3 multi-layer measurements with a traditional 2-layer big leaf resistance model.

Nomenclature

$\chi(z,t)$	= simulated NH_3 concentration (mol cm^{-3});
$\chi_c(z,t)$	= effective canopy compensation point concentration (mol cm^{-3});
$\chi_g(t)$	= soil compensation point concentration (mol cm^{-3});
$\chi_s(z,t)$	= stomatal compensation point concentration (mol cm^{-3});
$\chi_a(t)$	= measured NH_3 concentration @ $z=H$ (mol cm^{-3});
$\chi_0(z)$	= NH_3 concentration @ $t=0$ (mol cm^{-3});
$\rho(z,t)$	= air density (mol air cm^{-3});
$K_v(z,t)$	= scalar turbulent eddy diffusivity (cm^2 s^{-1});
$LAD(z)$	= leaf area density (cm^2 cm^{-3});
$v_c(z,t)$	= canopy exchange coefficient = $1/r_b(z,t)$ (cm s^{-1});
$v_s(t)$	= soil/litter layer exchange coefficient (cm s^{-1});
$r_b(z,t)$	= leaf quasi-laminar boundary layer resistance (s cm^{-1});
$r_s(z,t)$	= stomatal resistance (s cm^{-1});
$r_w(z,t)$	= cuticular resistance (s cm^{-1}); and,
H	= height of the top of the model domain (cm).

Preliminary Simulation Results

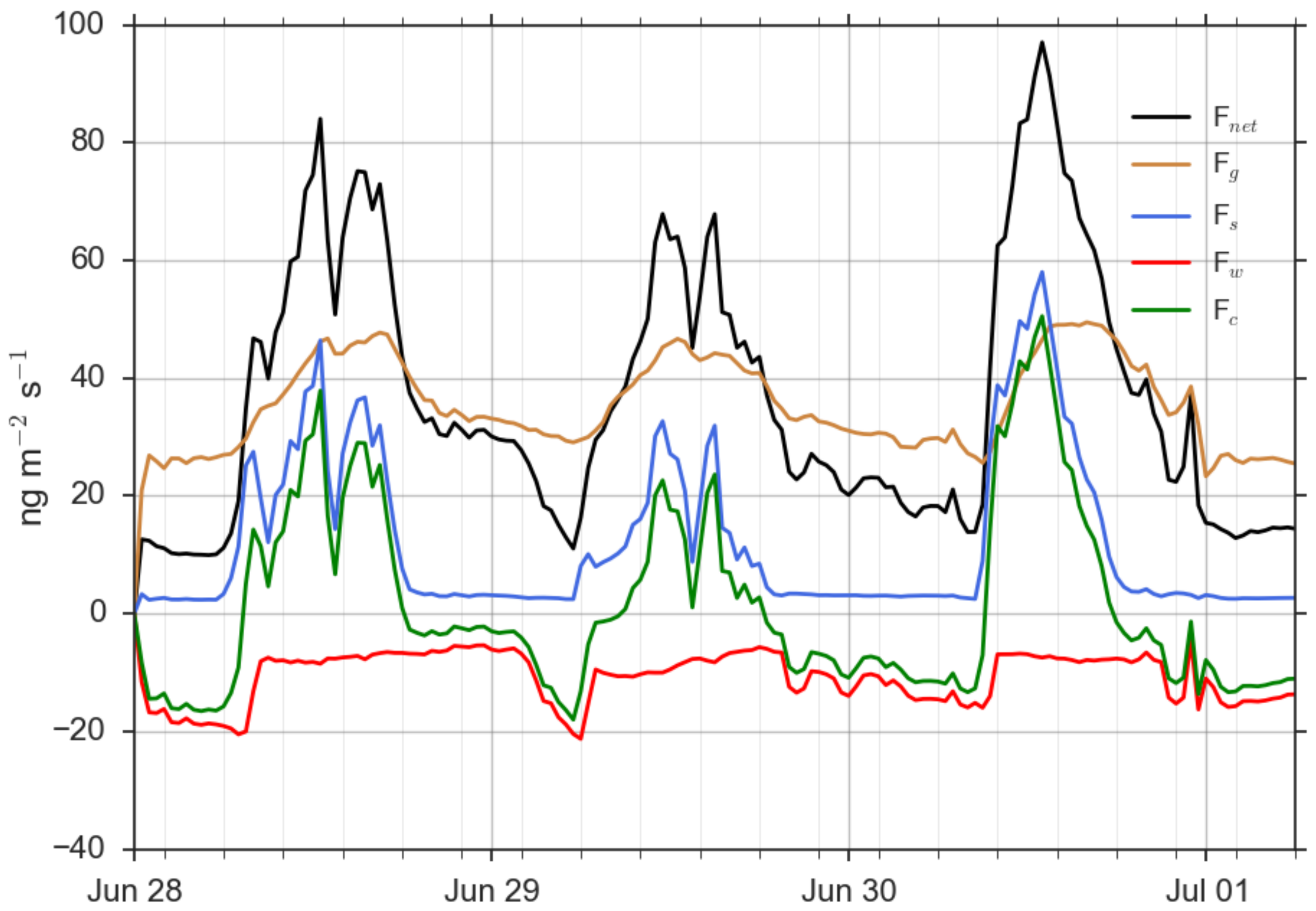

Figure 3. Simulated fluxes (ng m^{-2} s^{-1}) for June 28 to July 1, 2014. F_{net} = net above-canopy flux; F_g = flux from soil; F_s = stomatal flux; F_w = cuticular flux; F_c = effective canopy flux.

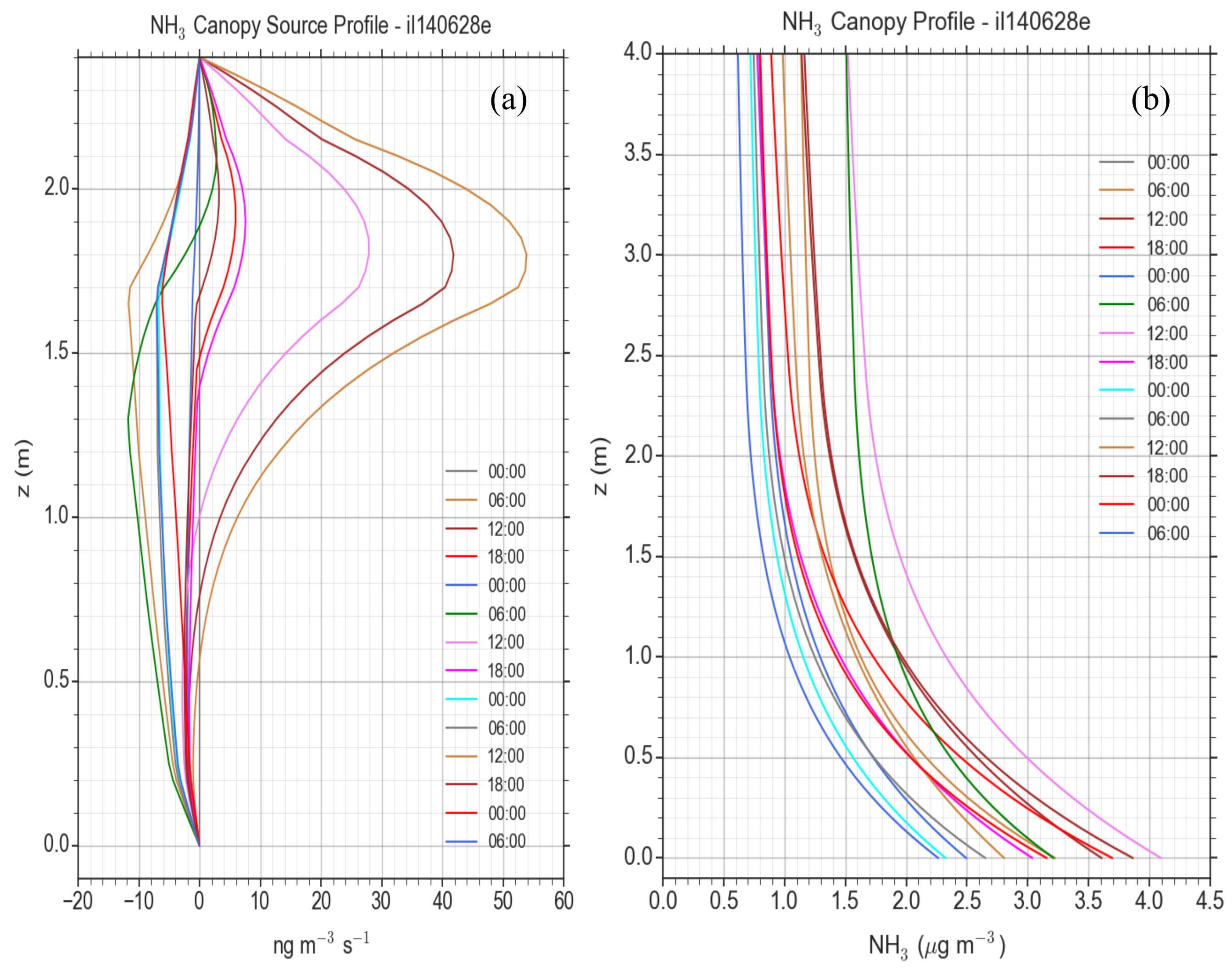

Figure 4. Simulation of June 28 to July 1, 2014: (a) Simulated canopy source/sink profiles (ng m^{-3} s^{-1}); (b) NH_3 concentration profiles throughout the domain.

Future Work

- Continued analysis of simulation results over entire growing season with comparison to measured fluxes.
- Sensitivity simulations to determine variability of results as a function of estimated soil and stomatal emission potentials.
- Comparison of ACCESS-NH3 results with a traditional 2-layer big leaf resistance model and with other models as available.

References

Greaver et al. (2012) Front. Ecol. Environ., 10, 365-372.
Ivanov et al. (1995) Ag. & Forest Meteorology, 75, 85-102.
Lichiheb et al., in preparation.
Nelson et al. (2017) Ag. & Forest Meteorology, 239, 202-212.
Pope and Dockery (2006) J. Air & Waste Manage. Assoc., 56, 709-742.
Saylor (2013) Atmospheric Chemistry & Physics, 13, 693-715.
Xing et al. (2013) Atmospheric Chemistry & Physics, 13, 7531-7549.

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