The effect of in-canopy chemistry on modifying biosphere / atmosphere exchange of air pollutants

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Project background

The biosphere / atmosphere exchange of many important reactive trace compounds is heavily modified by chemical conversions near and within plant canopies: NO emitted from soils is partly converted to NO_2 by reaction with O_3 which (unlike NO) can be taken up the overlying canopy, effectively reducing NO emission by up to 95%. Volatile NH_4NO_3 aerosol evaporates within warm canopies, converting slowly depositing aerosol compounds into rapidly depositing NH_3 and HNO_3, enhancing N deposition with consequences for vulnerable ecosystems. Finally, biogenic volatile organic compounds undergo many reactions that require consideration to quantify BVOC emissions more accurately, but also to understand their degradation and role in ozone and secondary organic aerosol production.

Such reactions are driven by a combination of long residence times and strong gradients in concentrations and meteorological drivers (temperature, relative humidity, radiation) near the ground that cannot spatially be resolved by typical chemical transport (CTMs) and coupled chemistry-climate models (CCMs). Existing empirical correction factors do not mechanistically respond to changes in turbulence, canopy structure, chemical climate and meteorological parameters and are therefore unsuited for extrapolating the effect into the future.

Therefore, a 1-dimensionsal modeling framework (ESX) has recently been developed within the European FP7 ECLAIRE project, for the simulation of the coupled processes of plant exchange, vertical transport and chemistry. This modular and scalable model is designed to become a depository of the state-of-the-art of surface / atmosphere modeling, from which simplified modules for the application in CCMs/CTMs can be derived, while remaining verified against the 'master version'. It is designed to interface with the EMEP CTM, which is used to underpin European policy within UNECE/CLRTAP.

This studentship will use the offline version of the model (a) to assimilate existing flux measurements of single species to derive ESX-compatible parameterisations for the application in CCMs and (b) to test its chemistry against existing comprehensive datasets of concentration and fluxes of interacting species. It will use the coupled CCM-ESX model to quantify the effect of in-canopy chemistry at the European scale.

Key research questions

1. To what extent is the surface / atmosphere exchange of reactive trace gases (NO_x, NH_3, HNO_3, VOCs) and aerosol components (e.g. NH_4NO_3) modified by in-canopy chemical processes?
2. How does the importance of in-canopy chemistry change between ecosystems and with chemical and meteorological climate?
3. To what extend do flux measurements made above plant canopies need to be corrected for chemical loss / production inside the canopy in order to derive the true exchange with the vegetation?
4. To what extent can the mechanistic coupled 1D model be simplified to be computationally efficient while still adequately reproducing the effect?

Methodology

Year 1	- Training in the science of surface / atmosphere exchange - Training in LINUX and FORTRAN programming environment - Training in running the ESX offline version - Summarise in-canopy turbulence measurements to improve in-canopy transport description for ESX, comparison against measurements - Paper 1 on evaluation and improvement of in-canopy transport description
Year 2	- Use of ESX to simulate existing flux measurements of NH_3; refining of model parameters against flux measurements - Sensitivity analysis of effect of model resolution on results - Run model for a number of measurement campaigns of combined flux measurements of NH_3, HNO_3 and NH_4NO_3 to validate thermodynamics and model description. - Paper 2 on effect of in-canopy thermodynamics on fluxes in the NH_3-HNO_3-NH_4NO_3 system across example sites - Presentation of results at an international conference (e.g. EGU)
Year 3 – 3.5	- Training in running the EMEP CTM - Development of a simplified approach to modelling the NH_3-HNO_3-NH_4NO_3 equilibrium in the coupled EMEP-ESX framework - Quantification of the importance of the effect at the European scale, sensitivity runs and under future climate - Presentation of results at an international conference (e.g. AGU) - Paper 3 on European modelling - Completion of write-up

While this is provides a comprehensive and achievable programme of research, there are many other aspects of ESX that could be developed, tested and applied for upscaling, and the student will have considerable opportunity to steer their own research programme, in response to personal interests and abilities. While the current programme is written to focus on NH_3 exchange and chemistry, the student might chose to focus on NOx chemistry or VOC/SOA chemistry instead.

Training

A comprehensive training programme will be provided comprising both specialist scientific training and generic transferable and professional skills in both University of Edinburgh and in NERC CEH. Professional skills includes a programme focused on personal effectiveness, communication, and career and project management, literature searching, presentations, and thesis writing. The student will also receive training in undergraduate laboratory demonstrating and project supervision. The student will attend relevant atmospheric science courses available in the UoE Schools of GeoSciences. It is envisaged that the student will attend appropriate summer schools (e.g. NCAS Climate Modelling summer school, Atmosphere Modelling Summer School in Lund) depending on availability, and we will apply for funding for the European ERCA (European Research Course on Atmospheres) School.

Requirements

Essentials: A minimum 2:1 undergraduate or a Master's degree in a physical science (Physics, Chemistry, Environmental Science, Environmental Engineering, Mathematics), highly numerate with experience in computer programming (ideally in Fortran).

Desirable: Knowledge of atmospheric physics, chemistry and/or numerical modelling.

References

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