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Accounting for surface hydric and thermal conditions in a volatilisation model

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Fertilisation and pesticide application to agricultural fields lead to the volatilisation of chemical compounds to the atmosphere. This results from a combination of physical and chemical processes occurring at the soil surface, leading to the release of gaseous species from the surface to the atmosphere. A mechanistic model, Volt'Air (Génermont and Cellier, 1997), has been developed to simulate these processes in order to eventually determine the amount of compounds - in our field of application, ammonia and pesticides - emitted from the surface to the atmosphere and its variation with time at hourly timescale.

The processes leading to volatilisation are highly dependent on local conditions, at the soil surface, namely surface temperature and moisture. Therefore, modelling volatilisation requires a precise representation of the soil surface temperature and water content and their dynamics at an appropriate time step. This requires an accurate modelling of the energy budget of the surface as well as the water and heat transfers beneath it. Especially, the model should be able to simulate some extreme desiccation events that can affect temporarily the topsoil (first few millimetres). Therefore, it is required to describe realistically the heat and water fluxes at an hourly time scale in soil layers of few millimetres near the soil surface to simulate correctly the volatilisation of a chemical compound applied to the field.

The goal of this work is to determine if the aforementioned representation by the ammonia and pesticides emission model Volt'Air is accurate enough.
To test the model, we used two datasets of volatilisation measurements on open field,

including the energy budget main variables. Some discrepancies between measured and simulated volatilisation fluxes of chemical compounds have been observed, which could be attributed to an inadequacy in the processes formulations. Moreover, some variables are quite difficult to measure precisely, as obtaining normalized samples of surface layers of a few millimetres is not straightforward. Thus these data sets do not provide a reliable assessment of the surface water content for our tests.

Therefore, either to gain access to specific variables or to attempt to explain discrepancies in Volt'Air, we used the soil-atmosphere transfer model SiSPAT (Braud et al., 1995) as a reference model. SiSPAT makes a full coupling between heat and water transfers in the soil while VoltAir does not.

SiSPAT outputs were firstly compared to the same observed data as Volt'Air, like surface temperature, components of the energy budget or water content of the different layers of the soil profile. We also had access to data sets of evaporation for several types of soil to further test the behaviour of both models against the measurements. Secondly, some more precise SiSPAT outputs were used as reference for the further evaluation of Volt'Air.

Analysing this comparison allows us to identify the possible weaknesses of the Volt'Air model from the main differences with SiSPAT processes formulation. For example, the two models use different pedotransfer functions to establish the water potential and conductivity inside the soil matrix. The analysis will also concern the boundary conditions, which are differently prescribed in the two models.

Braud, I., A. C. Dantasantonino, et al. (1995). "A Simple Soil-Plant-Atmosphere Transfer Model (Sispat) Development and Field Verification." Journal of Hydrology **166**(3-4): 213-250.

Génermont, S. and P. Cellier (1997). "A mechanistic model for estimating ammonia volatilization from slurry applied to bare soil." Agricultural and Forest Meteorology **88**(1-4): 145-167.