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Identification of sensitive parameters in the modeling of SVOCs reemission processes from soil to atmosphere

Vincent Loizeau (1,2), Philippe Ciffroy (3), Luc Musson Genon (1,2), and Yelva Roustan (1)

(1) CEREA, Joint Laboratory Ecole des Ponts Paristech/EDF R&D, 77455 Marne la Vallée, France (vincent.loizeau@edf.fr), (2) MFEE, EDF R&D, 6 quai Watier 78401 Chatou, France, (3) Laboratoire National d'Hydraulique et Environnement, EDF R&D, 6 quai Watier 78401 Chatou, France

Many studies have shown that semi-volatile organic compounds (SVOCs) are subject to Long-Range Atmospheric Transport (LRAT) and that such a transport may occur through a series of deposition-reemission events at the soil surface-air interface. This periodic movement of pollutants between soil and atmosphere is called the 'grasshopper effect'. Thus, it appears necessary to take into account the exchange between soil and atmosphere to properly simulate the fate of these pollutants at regional or global scale. The prediction of reemission from soils is however associated with large uncertainties, which can be schematically classified into three main sources : (i) natural variability, including nature of soil (organic matter content, porosity, water content) and meteorological conditions ; (ii) uncertainty about intrinsic properties of chemicals, like degradation rate or partitioning between environmental components, which govern the dynamics of chemicals in air and soils ; (iii) model structure, and particularly the discretization of soil compartment.
Considering this background, a major challenge is to identify the most sensitive sources of uncertainty in modelling the reemission of chemicals from soils, in order to know where the priority has to be set for upgrading SVOC dispersion estimation.

To answer this question, we studied a multi-layer soil model, including exchanges between soil and atmosphere. A sensitivity analysis was conducted by affecting probability density functions for each of model parameters. Four chemicals were selected (Benzo(a)Pyrene, PCB-28, Lindane and Hexachlorobenzene) because of their contrasted behaviors in soils, as expected by their partition and degradation properties. For this first exercise, simple emission scenarii were considered, i.e. a period of constant concentration in air (where realistic concentrations were estimated for each chemical from monitoring data provided by EMEP) followed by a zero-concentration in air. Although these scenarii are obviously simplified, they were selected to identify sensitive parameters in two extreme conditions, i.e. constant emission in the atmosphere over a long period, and follow-up of ban regulation.

Results show that the rank of sensitive parameters depends on the intrinsic properties of the investigated substances, in particular on their mobility potential in soils and their ability to volatilize. Despite such differences, general patterns can however be observed: for all the substances, organic matter content in the soil is one of the most sensitive parameters in the simulation of reemission fluxes in both contamination conditions (i.e. charge and discharge periods). Instead, the number of layers used in the model for simulating the transfer of pollutants in the soil profile is less influential. These results allowed defining priorities in LRAT modeling strategy, highlighting in particular that mapping organic matter in soils instead of using a generic value could significantly improve the reemission estimation.