EGU22-1962
https://doi.org/10.5194/egusphere-egu22-1962
EGU General Assembly 2022

Modeling the translocation and transformation of chemicals in the soil-plant continuum: a dynamic plant uptake module for the HYDRUS model

Giuseppe Brunetti[1], Jirka Šimůnek[2], and Radka Kodešová[3]
[1]Institute for Soil Physics and Rural Water Management, University of Natural Resources and Life Sciences, Vienna, Austria (giuseppe.brunetti@boku.ac.at)
[2]Department of Environmental Sciences, University of California, Riverside, USA (jsimunek@ucr.edu)
[3]Department of Soil Science and Soil Protection, Czech University of Life Sciences, Czech Republic (kodesova@af.czu.cz)

Soil pollution from neutral and ionizable compounds poses a significant threat to water resources management and food production. The development of numerical models to describe their reactive transport in the soil-plant domain is of paramount importance to elaborate mitigation strategies. However, most existing models simplify the description of physicochemical processes in soil and plants, mass transfer processes between soil and plants and in plants, and transformation in plants. To fill this scientific gap, we first coupled the widely used hydrological model, HYDRUS, with a multi-compartment dynamic plant uptake model, which accounts for differentiated multiple metabolization pathways in plant's tissues. The model, which is able to simulate the reactive transport of neutral compounds, has been successfully validated against experimental data, and integrated in the Graphical User Interface of the HYDRUS software suite. To further extend its domain of applicability, we have recently adapted its theoretical framework to simulate the translocation of ionizable compounds. The new modeling framework connects a biophysical multi-organelles model to describe processes at the cell level with a semi-mechanistic soil-plant model, and accounts for dissociation processes and electrical interactions with cell biomembranes. Validation against experimental data showed encouraging results and opens new perspectives for its use for predictive and explanatory purposes.

References

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