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Modelling the fate of the natural toxin ptaquiloside at pedon-scale. From plant to groundwater.

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Natural toxins, i.e. toxins produced by living organisms, are getting increasing attention as emerging pollutants. Some natural toxins are highly toxic exceeding the toxicities of common industrial chemicals, such as pesticides. Also natural toxins may be produced in high amounts and they may be released continuously from the organism to the environment. The hazard of natural toxins toward humans is determined by the physicochemical characteristics of the toxins, their loads and fate in the environment. Modelling the fate and transport of natural toxins presents several challenges and unknowns compared with modelling of anthropogenic pollutants. Thus the physicochemical characteristics, biological production dynamics and the release mechanisms are seldomly well quantified. In case of plant toxins the release may be highly variable both in time and space. The aim of this work is to develop a conceptual approach for modelling the fate and leaching of plant toxins. Our work focus on ptaquiloside (PTA), which is a carcinogenic compound produced by bracken fern (Pteridium aquilinum) in high amounts. Ptaquiloside is a hydrophilic and non-sorbing sesquiterpenoid, which in most cases degrades rapidly by microbes and abiotic hydrolysis. Degradation of PTA in the soil is highly dependent on depth (microbial activity), pH and temperature. Half-lives of PTA in different soil horizons at 10 0C has been estimated from 3.3 to 105 days. In this work, we introduce a novel approach for modelling natural toxins in the environment by incorporating a new process for the generation of PTA in the plant, release of PTA from the plant by wash-off via precipitation, PTA recovery in the plant after wash-off and a separate function for PTA hydrolysis. These functions have been implemented into DAISY, a soil-plant-water-atmosphere model. The parameterization of the model is developed from field data and lab experiments. At a first step, the results of this study are compared against experimental data from canopy to the soil surface. Additional analyses show that the largest uncertainties in the model are the toxin production in the plant, spatial and temporal variability of toxin content, and specially the transfer from the plant to the soil surface.