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MODELLING THE FATE OF IONIZABLE TRACE ORGANIC CHEMICALS FROM CONSUMPTION TO FOOD CROPS

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Summary: In this study, we developed and applied a simulation tool to comprehensively predict the fate of three ionizable trace chemicals (triclosan—TCS, furosemide—FUR, ciprofloxacin—CIP) from human consumption/excretion up to the accumulation in wheat, following application of sewage sludge or irrigation with river water. Highest translocation to wheat (4.3 µg kg_{DW}^{-1} in grain) was calculated for FUR, being more significant with irrigation (>45% of emission to soil) than with sludge application (<30%). The simulation tool presented here can be used for estimating human exposure to trace chemicals via food crop intake and for priority setting among emerging pollutants.

Keywords: fate modelling of ionizable trace chemicals; wastewater treatment; plant uptake

Introduction. Trace organic chemicals released by human use (e.g., pharmaceuticals and biocides) are incompletely eliminated in municipal wastewater treatment plants (WWTPs) and thus released to surface water via treated effluents. Emissions to agricultural soils further occur as a result of fertilization with sewage sludge—a practice recommended by the Sewage Sludge Directive —or irrigation with freshwater or treated WWTP effluent (Ternes et al., 2007), resulting in the potential accumulation in food crops. Fate models can be used to assess human exposure to trace chemicals via food crop intake (Prosser et al., 2014) and to support pre-screening of potentially hazardous chemicals. The main objective of this study was to develop a simulation tool to predict the fate of three ionizable trace chemicals (TCS, FUR, CIP) from household consumption to the accumulation in winter wheat, following release to soil via sludge application or freshwater irrigation (Fig. 1).

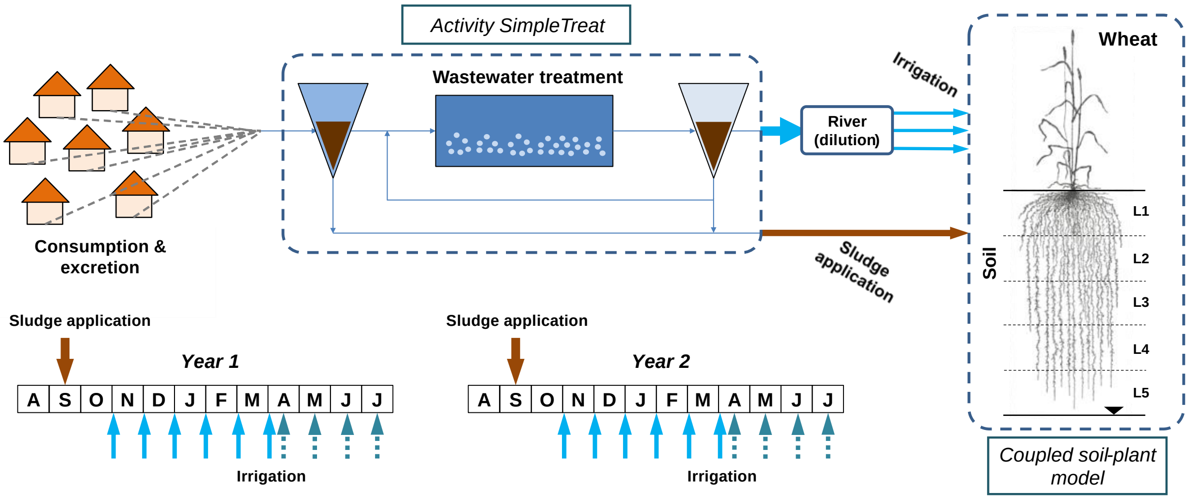

Figure 1. System boundaries for fate prediction of TCS, FUR and CIP from consumption to uptake into winter wheat.

Materials and Methods. The simulation tool was developed by combining a model for fate prediction in WWTPs (Activity Simple Treat, Franco et al., 2011) and a dynamic soil-plant uptake model previously parameterized for winter wheat (Legind et al., 2012). The simulation tool was tested for selected geographical scenarios (Germany, Sweden, Denmark, Italy) by using country-specific (e.g., consumption/emission rates, precipitation and temperature) input data. Dynamic plant uptake in wheat tissue (roots, stem, leaves, grains) was simulated for a period of two years (Fig. 1), with sludge application occurring in mid-September and irrigation in November–April (Italy) or April–July (Denmark). A Monte Carlo-based approach was considered to account for the uncertainty associated to physico-chemical (e.g., ionization constant pK_a) and biokinetic model parameters (e.g., biotransformation rate in activated sludge k_{bio}) from literature.

Results and conclusions. Results obtained suggest limited removal of FUR during wastewater treatment (≤40%) and significant accumulation of TCS and CIP in sewage sludge (1.4–2.9 mg kg_{DW}^{-1}) as compared to FUR (0.02–0.11 mg kg_{DW}^{-1}). Significant translocation to wheat was predicted for FUR, with concentrations up to 54.1 µg kg_{DW}^{-1} in roots. Irrigation, occurring more in proximity to plant harvest, was found to enhance translocation of FUR to whole wheat plant (48.9% of emission to soil) as compared to sludge application (27.6%) (Fig. 2a). Bioconcentration factors to grain (BCF_{grain}) were calculated to assess the relative translocation from soil to this compartment:

$$BCF_{grain} = \frac{C_{grain}(harvest)}{C_{soil}(amendment)}$$

where C_{soil}(amendment) identifies the concentration in soil at sludge application or at the last irrigation pulse. Highest BCF_{grain} values (> 10 kg_{DW} kg_{DW}^{-1}) were predicted for FUR, while TCS and CIP exhibited negligible uptake into grain (BCF_{grain} < 0.1 kg_{DW} kg_{DW}^{-1}).

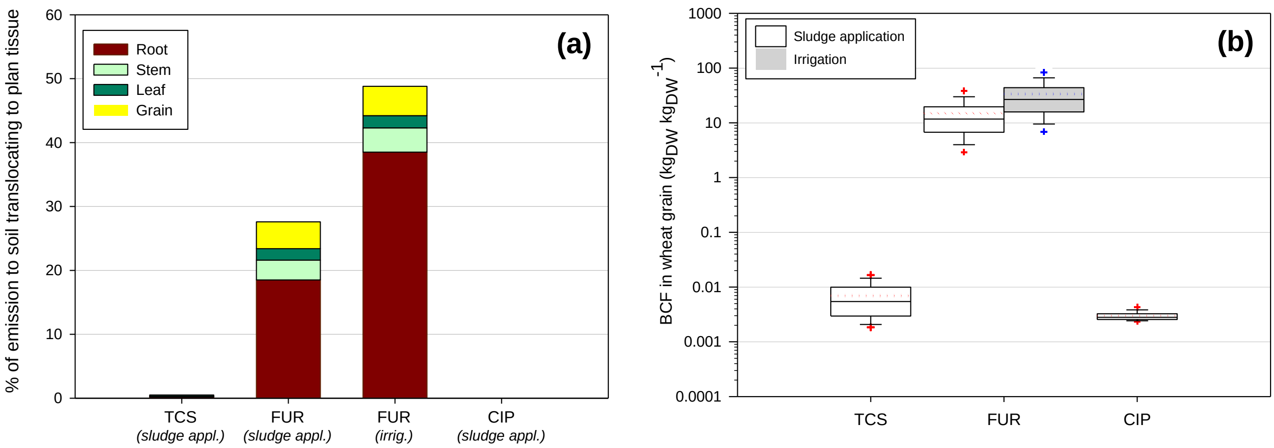

Figure 2. Predicted relative translocation to wheat tissues (a) and bioconcentration factors (BCFs) in grain (b) for TCS (Denmark, sludge application), FUR (Denmark, irrigation and sludge application) and CIP (Italy, sludge application)

Model predictions reveal the potential for FUR to be uptaken by winter wheat. FUR is a weak acid, thus exhibiting little adsorption in soil and good translocation to plants. The simulation provides for an upper estimate, as *in planta* degradation is neglected. No data for the geographical areas assessed were found to validate the predictions. Overall, the proposed simulation tool can track the fate of ionizable trace chemicals from human emissions through WWTPs into food crops, offering the possibility for estimating human exposure via dietary intake. For further details, the reader is referred to Polesel et al. (2015).

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