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Modelling the fate of ionizable trace organic chemicals from consumption to food crops

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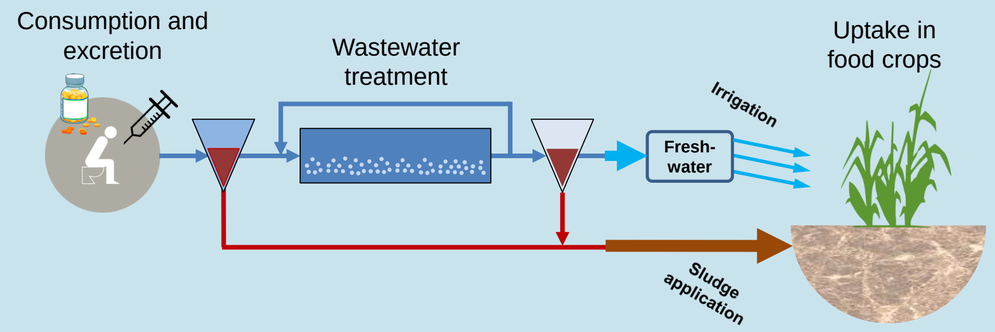
Introduction

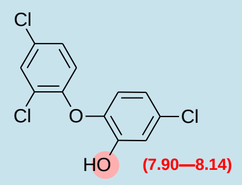
Background

Excreted pharmaceuticals and biocides undergo incomplete removal in urban wastewater treatment plants (WWTPs), thus persisting in effluent and sludge [1,2]. Residual amounts are released to agricultural systems via biosolids application and irrigation with freshwater or treated effluent, eventually resulting in the uptake of trace chemicals into food crops [3–5].

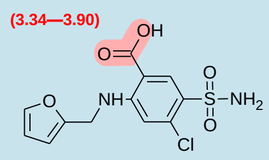
Objectives

- To develop and test a **simulation tool** for fate prediction of widely used trace organic chemicals (TCS, FUR, CIP) **from household consumption to the uptake into food crops (winter wheat)**
- To assess the **propagation** of input **uncertainty** (e.g., degradation rates of chemicals) to model output
- To evaluate **differences in uptake into winter wheat** due to:
  - **Biochemical properties** of ionizable trace organic substances
  - **Emission pathways** (fertilization, irrigation) to agricultural systems

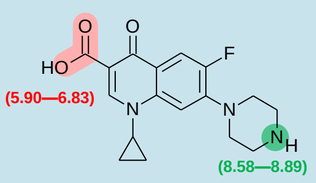




Triclosan (TCS)



Furosemide (FUR)



Ciprofloxacin (CIP)

Modelling approach

Models: A simulation tool was developed combining the WWTP model *Activity SimpleTreat* [6] and a *Dynamic plant uptake model* [3,7]. Both models allow for fate prediction of ionizable chemicals. Regional consumption/emission data (EU) for TCS, FUR and CIP were used.

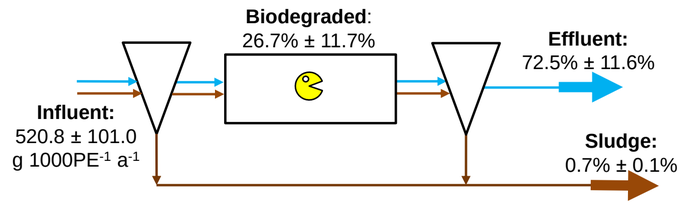
System boundaries: WWTP emissions to agricultural systems were assumed to occur via two-year sludge amendment and freshwater irrigation. Uptake in wheat was determined at harvest (second year).

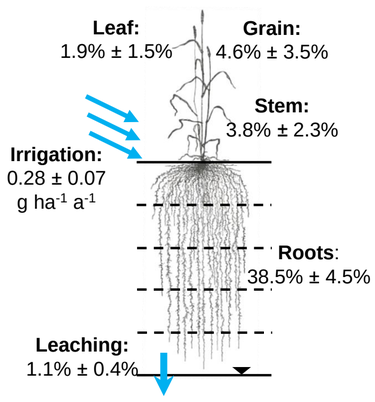
Uncertainty analysis: Based on literature data variability, parameter distributions were defined for relevant input (see table). Uncertainty propagation to model output was derived using Monte Carlo method.

Parameter	Mean value (for TCS)	Input uncertainty (U=uniform distribution)
Excretion rate (-)	60%	± 30% (U)
Half-life in soil (d)	13–110	Range min–max

Fate predictions – The case of FUR

In the figure below, we present fate predictions for FUR based on consumption data for Denmark, considering release to soil via irrigation. Reported standard deviations refer to the uncertainty propagating from model input.

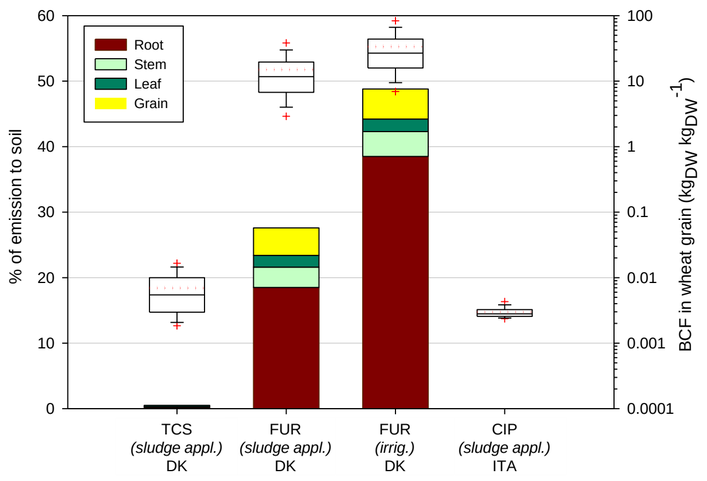




Model predictions show limited FUR removal in WWTP, with most of influent load (> 60%) released with effluent and negligible accumulation in sewage sludge. Significant FUR uptake in wheat was predicted following irrigation (48.9 ±5.4% of emissions). Accumulation in wheat grain (4.6±3.5%) likely resulted from ion trapping in phloem (pH=8) [8].

Uptake into winter wheat

Limited uptake in wheat (<1% of emissions) was predicted for TCS and CIP. Irrigation, occurring in proximity to harvest, increased FUR uptake in wheat (48.9% of emissions) compared to sludge application (27.6%). Bioconcentration factors were calculated for wheat grain:

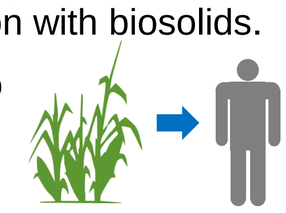


$$BCF_{grain} = \frac{C_{grain}(harvest)}{C_{soil}(amendment)}$$

Highest BCF_{grain} (> 10 kgDW $kgDW^{-1}$) was predicted for FUR, as for other polar anionic trace chemicals [5]. Significant uncertainty was overall associated to BCF_{grain}.

Conclusions and future perspectives

- Among the three chemicals assessed, **FUR** was predicted to be the most persistent in WWTPs and to significantly accumulate in winter wheat (30%–50% of emission to soil).
- **Irrigation** can **enhance the relative uptake** of trace chemicals in wheat as compared to fertilization with biosolids.
- The developed simulation tool can be used to estimate human exposure to trace chemicals via **dietary intake** of wheat grain products.



- Findings from this study **encourage field investigations** on the fate of trace chemicals (e.g., FUR) **in agricultural systems**, for which evidences are still limited.

For further details

References: [1] Ternes TA 1998, Water Res. 32, 3245–60. [2] Bester K 2003, Water Res. 37, 3891–6. [3] Prosser RS et al. 2014, Environ. Toxicol. Chem. 33, 975–84. [4] Calderón-Preciado D et al. 2011, Water Res. 45, 221–31. [5] Goldstein M et al. 2014, Environ. Sci. Technol. 48, 5593–600. [6] Franco A et al. 2011, Available at homepage.env.dtu.dk/stt/ [7] Legind CN et al. 2012, PLoS One 7, e47002. [8] Trapp S 2004, Environ. Sci. Pollut. Res. 11, 33–39.

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From consumption to harvest: Environmental fate prediction of excreted ionizable trace organic chemicals

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