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Simulation of pharmaceuticals in the environment

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1. Introduction

Pharmaceuticals are high-volume compounds with special concern which do not fall under the EU legislation REACH. Environmental risk was investigated within the EU FP 7 project PHARMAS. Our objective was to estimate indirect human exposure via the exposure routes from wastewater to rivers and to agricultural soils, and further via bioaccumulation in fish and crops to humans, using a system of coupled mathematical simulation models. The study concentrates on antibiotics (and antitumor agents, not shown), which are generally ionizable chemicals (mostly cations and zwitterions). Ionizing chemicals undergo a variety of processes not seen for neutral compounds, like dissociation, electrical attraction, ion trap, adsorption to proteins. Their partition behavior is thus only partly governed by lipophilic interactions (as described in existing models), but often dominated by ionic interactions. This means existing and established model systems required update and modification to run satisfactorily for these types of compounds. The simulated system is shown in Figure 1.

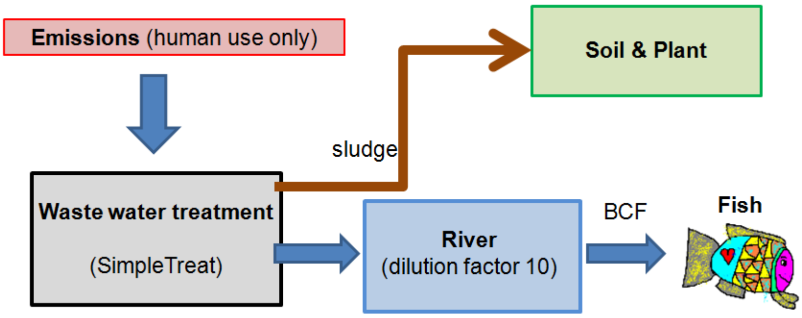

Figure 1: System of simulation models for indirect human exposure to pharmaceuticals in the environment.

2. Materials and methods

Use data of drugs in Denmark from medstat.dk corrected for metabolism in human body were used as input data. Environmental conditions were set typical for Denmark. Fate in wastewater treatment plant was simulated with a modified SimpleTreat model [1]. Concentrations in rivers were calculated with the common dilution factor 10. The bioconcentration factor fish was estimated with a dynamic cell model based on the Fick-Nernst-Planck equation [2,3]. A novelty is the introduction of adsorption to proteins into the BCF model. The adsorption to proteins was found to be the dominant partition process for polar electrolytes and in particular for zwitterions.

A validated simulation model considering transfer of water and solutes from soil to plant and leaching to groundwater [4] was adopted and reprogrammed for ionic compounds [2]. Input of pharmaceuticals to the field was with sewage sludge application (7 t/m^2/a) and by irrigation. If not available from measurements, the adsorption to soil was estimated using recently developed Koc-prediction methods for acids and bases [5]. The partitioning into plant tissue was calculated with the cell model, too (though, with different parameterization), and integrated into the dynamic model. Figure 2 shows a sketch of the models employed for simulations.

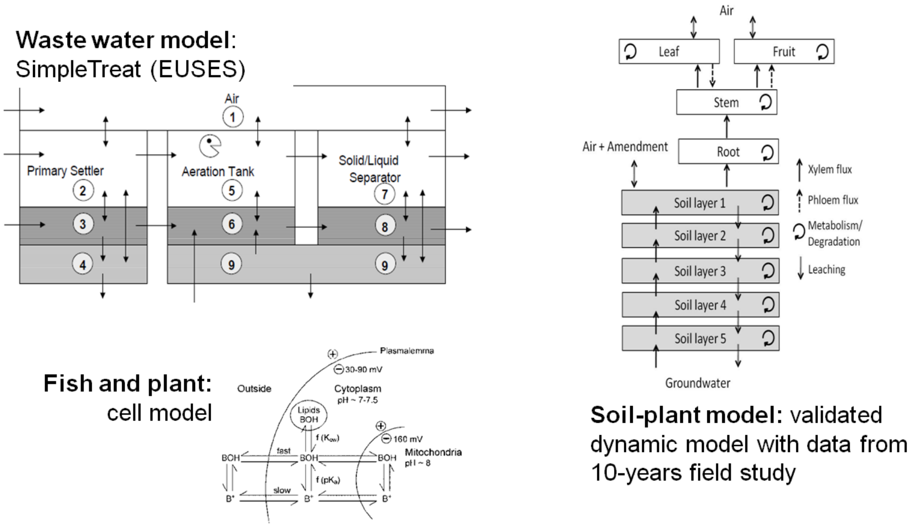

Figure 2: A sketch of the model approaches used to simulate emissions via wastewater, bioconcentration in fish, concentration in soil, leaching and plant uptake.

3. Results and discussion

3.1. Emissions and resulting concentrations

Highest human usage of antibiotics in Demark is for erythromycin, tetracycline, ciprofloxacin, doxycycline and trimethoprim (200 to 600 g/1000 inh/ year). All except erythromycin which is rapidly degraded adsorb strongly to sewage sludge, with resulting concentrations > 1 mg/kg. Such high concentrations of antibiotics in sewage sludge have been confirmed repeatedly by chemical analysis. Predicted concentrations in effluent and river water are much lower (max 100 ng/L). In Denmark, 60% of sewage sludge are applied to agricultural land, and calculated concentrations of some antibiotics in top soil > 10 μg/kg can result.

The first results indicate that a couple of antibiotics show good plant uptake and that amendment of agricultural fields with sewage sludge leads to relevant human exposure. The comparison of measured data to simulation results at all stages (effluent water, sewage sludge, soil, plants) is satisfying. We will use this tool to predict environmental concentrations and dietary uptake of high-volume drugs.

4. Conclusions

Summarized, the major conclusions are

- this simulation system adopted to ionizable compounds can be used to predict emissions from wastewater, residues in soil and plant uptake of pharmaceuticals (and pesticides).
- dietary exposure to human antibiotics is higher with field crops than with (river) fish.
- uncertainties and variations (also of experimental data) are high.

5. References

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