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Polesel, Fabio; Plósz, Benedek; Trapp, Stefan

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DTU Environment
Department of Environmental Engineering

Technical University of Denmark

Activity-based fate modelling for risk assessment of three ionizable organic compounds (triclosan, furosemide, ciprofloxacin)

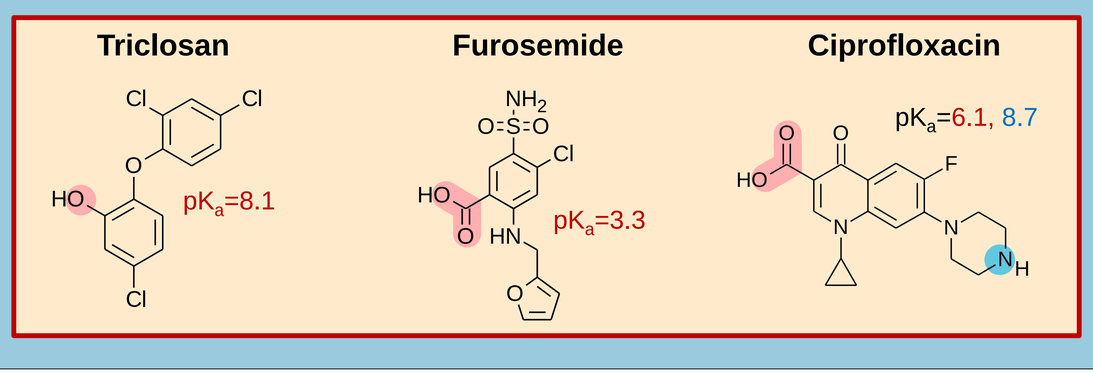
Fabio Polesel (fabp@env.dtu.dk), Benedek Gy. Plósz, Stefan Trapp

Department of Environmental Engineering, Technical University of Denmark, Bygningstorvet, DK-2800 Kgs. Lyngby, Denmark

Background and target substances

Most pharmaceuticals are ionizable compounds
Ionizable chemicals are 49% of all substances registered according to the REACH protocols [1]. 77.5% of pharmaceuticals assessed within a data set of over 500 substances were found to ionize at biologically relevant pH range [2].

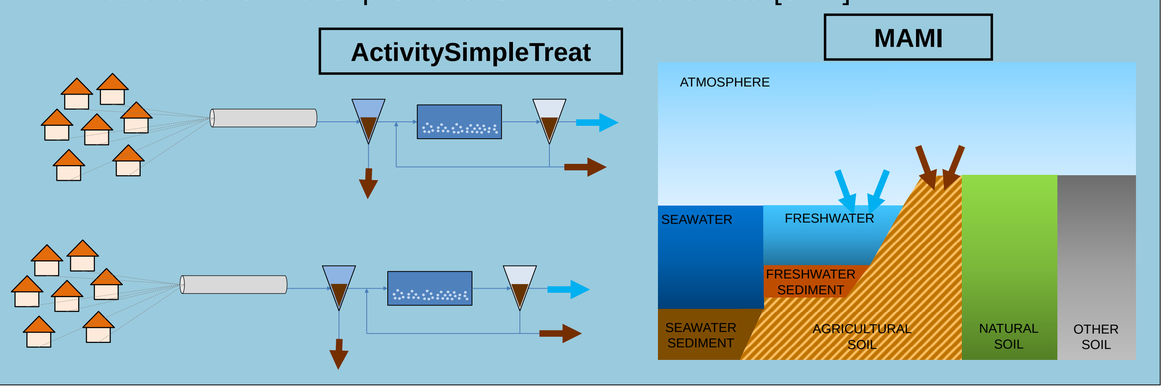
Prediction of the fate of ionizable chemicals: a novel approach
Activity-based models have been developed to predict the environmental fate of organic ionizable compounds, based on their QSAR properties [3,4].



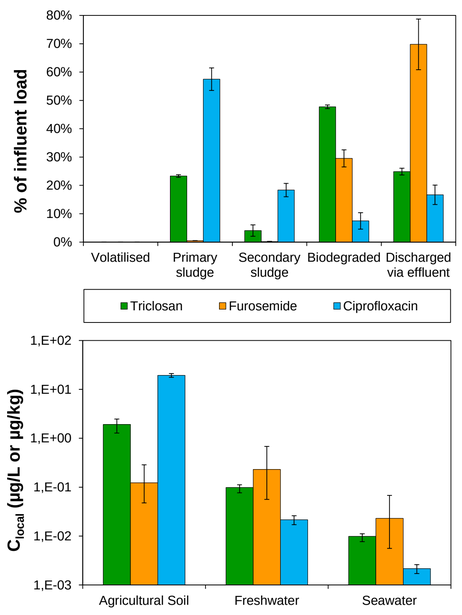
Objectives and Methods

Environmental risk assessment of three ionizable pharmaceuticals

- Prediction of fate according to **REACH** regulation: local (**C_{local}**) and regional concentrations (**$PEC_{regional}$**) of parent substances
- Combination of steady-state models for WWTP fate (**Activity SimpleTreat**) and regional fate (**MAMI-M**ultimedia **A**ctivity **M**odel for **I**onics) [3,4]
- Assessment of **real emission scenarios** (annual average): Lower Saxony, Southern Sweden, Denmark, Northern Italy
- **Validation** of model predictions with literature data [5-12]



Model predictions



WWTP fate predictions

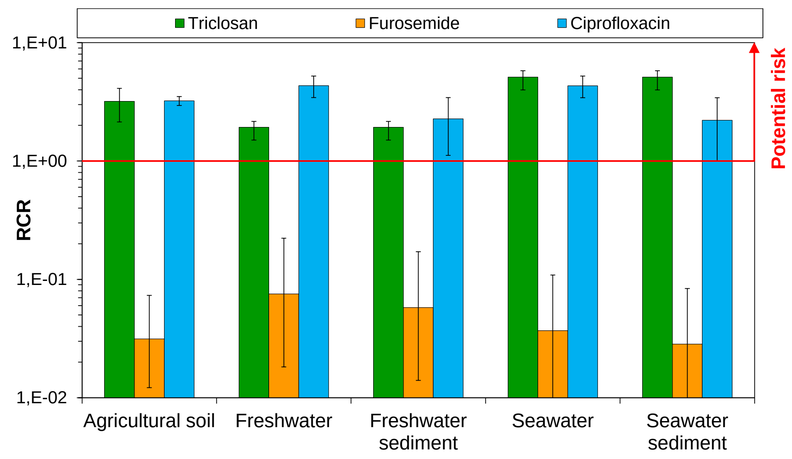
- Furosemide had the lowest removal (> 70% discharged via effluent).
- Triclosan was ~50% biodegraded and 25% discharged via effluent.
- Ciprofloxacin was mostly removed in the sludge (>70%) due to very high sorption coefficient.

C_{local} in receiving freshwater bodies were estimated to be ≥ 0.1 µg/L for triclosan and ciprofloxacin. Ciprofloxacin was also found to accumulate in soil (C_{local} > 10 µg/kg), as a result of sludge amendment.

$PEC_{regional}$ estimated with MAMI were found to be < 6% of C_{local} (not shown).

Risk characterization

PEC_{local} (by combining **C_{local}** and **$PEC_{regional}$**) were used to calculate **R**isk **C**haracterization **R**atios **(RCRs)**. **P**redicted **N**on-**E**ffect **C**oncentrations **(PNECs)** were defined from worst cases in literature or calculated according to REACH TGD. PNECs used were 53 ng/L (triclosan), 3.1 µg/L (furosemide), 5 ng/L (ciprofloxacin) in water and 0.6 µg/kg (triclosan) in soil.



$$RCR = \frac{PEC_{local}}{PNEC}$$

RCR > 1 was found for triclosan (1.9–5.1) and ciprofloxacin (2.2 –4.3). No potential risk was exhibited to furosemide (RCR < 0.2).

Validation

Results were compared with WWTP removal rates and concentrations in literature to test the **reliability of the models**.

Substance	WWTP removal			Concentrations in freshwater			
	Simulated	Literature	Ref.	Scenario	PEC_{local}	Literature	Ref.
Triclosan	**74%–76%** (46-48% degraded)	**55%–98%** (48% degraded)	[5,6]	Lower Saxony	80 ng/L	3–90 ng/L	[9,10]
Furosemide	**21%–33%**	**21%**	[7]	Denmark	680 ng/L	250–420 ng/L	[11]
Ciprofloxacin	**80%–87%** (70%–82% in sludge)	**88%** (83% in sludge)	[8]	Northern Italy	17–26 ng/L	14–26 ng/L	[12]

Conclusions

- **The modification of the standard fate models (SimpleTreat and Level III regional model) to multispecies models for ionizable compounds was possible and allowed prediction of acids' and zwitterions' fate.**
- **Model predictions of WWTP fate and of local concentrations were realistic.**
- **Potentially high risk at local level was associated to triclosan and ciprofloxacin in water, sediment and soil compartments in all scenarios assessed.**
- **Further investigation is needed, as fate is influenced by e.g., temporal variations of emissions and conjugates' retransformation [13,14].**

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In all the graphs presented, columns represent the mean value (of % of influent load, C_{local} and RCR) among all scenarios considered, and error bars refer to the range in which those values are included.