Modelling the fate of psychoactive compounds in groundwater at field scale (Berlin, Germany)

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Introduction

In Berlin, more than one century until 1980s, untreated wastewater was irrigated directly onto fields of sewage farms and led to accumulation of contaminants in the soil and ground water.

Several psychoactive compounds, including meprobamate, pyrithyldione, primidone, and its metabolites phenobarbital and phenylethylmalonamide are subjects of the present study.

Objectives

- Understand why the psychoactive compounds are still in the groundwater
- Estimate concentrations of the compounds in the sewage
- Identify field scale linear adsorption parameters (K_d)

Study Site

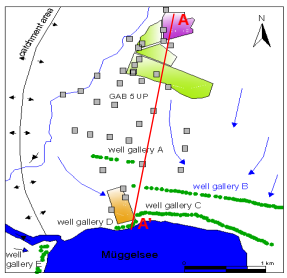


Fig. 1: Location map of studiy site (Meffe et al., 2011).

Entry Periods Psychoactive Compounds

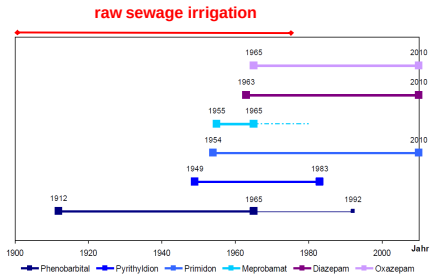


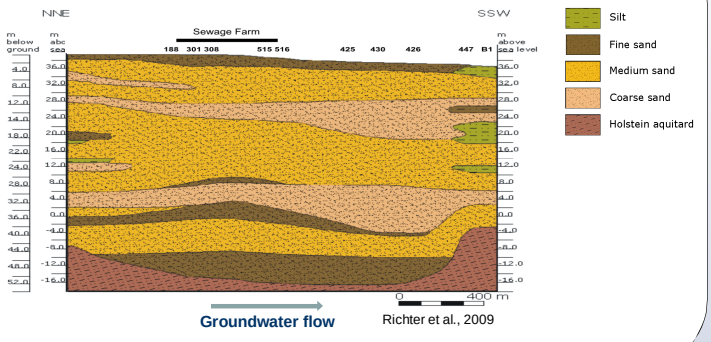
Fig. 2: Occurrence of psychoactive compounds on German market.

Modelling Information

2D Model

- Software: PMWIN8
- 2D flow and transport model (Hamann, 2008; Meffe et al., 2011)
- Simulation period from 1906 to 2016

Cross Section



Richter et al., 2009

Fig. 3: Cross section for 2D model.

Modelling Approach

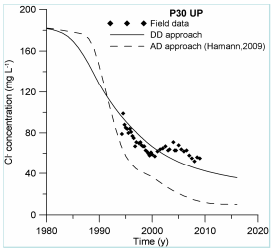


Fig. 4: Cl^- breakthrough curve at well P30 UP for the dual-domain and advection-dispersion approaches (Meffe et al., 2011).

- Dual-domain mass transfer approach.
- Concentration of psychoactive compounds in the irrigated wastewater was assumed constant during the time period they occurred on the German market

Modelled & Observed Data

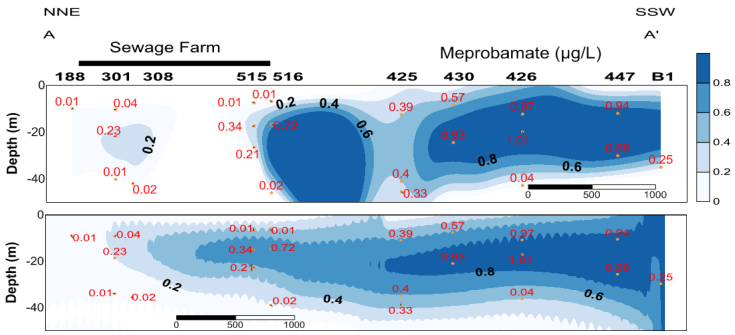


Fig. 5: Modelled and observed distribution of meprobamate along the transect A-A'

Modelled & Observed Data

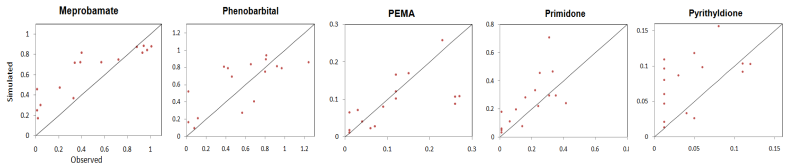


Fig. 6: Scatter plots for the comparison between modelled and observed data.

Preliminary Results

Compound	Calibrated concentration (µg/L)	Calibrated K_D (L/kg)
Meprobamate	32	0
Phenobarbital	15	0
Pyrithyldione	0.9	0
Primidone	2.2	0
Phenylethyl-malonamide	0.8	0

Conclusion

- Long-term persistence of detected psychoactive compounds in the groundwater results from non-equilibrium mass transfer between mobile and existing immobile pore water.
- Chemical adsorption plays an unimportant role for the retardation of these substances.

Acknowledgments

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References

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