Determination of transfer factors for solute concentrations from agricultural fields to drinking water abstraction points

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Abstract

The stepwise attenuation of solute concentrations has been determined, starting from the unsaturated zone underneath treated fields across the deeper aquifer, down to drinking water abstraction wells. The partial or overall transfer or attenuation factor may help to make informed decisions on the magnitude of the decrease in concentrations from shallow leachate to drinking water abstraction, which is largely caused by mixing. The test compound was N,N-dimethylsulfamide (DMS), a soil metabolite of the fungicides Dichlofluanid and Tolylfluanid, with no sorption and a moderate to long degradation half-life in soil. On average an overall 59-fold attenuation was observed (n = 3).

Introduction

For the determination of the attenuation factors three test sites in western and southern Germany were selected. Vertical transport below the treated area via leaching was simulated using the models PEARL and HYDRUS-(1D), transport in the saturated zone was calculated with HYDRUS-(2D) and FEFLOW. The results were validated with monitoring data from different locations across the transport pathway.

The calculated attenuation factors demonstrate for three real examples, how several influencing parameters like climatic conditions, cropping, soil conditions, catchment size, depth to groundwater and dilution in the aquifer affect the concentration of DMS in water in relation to distance and time. Despite the large variety in such properties, a quite similar behavior in terms of attenuation was demonstrated across these studies.

Using the test compound DMS ensures conservative estimates at the lower end of expected attenuation, due to its non-sorptive and quick transport behavior.
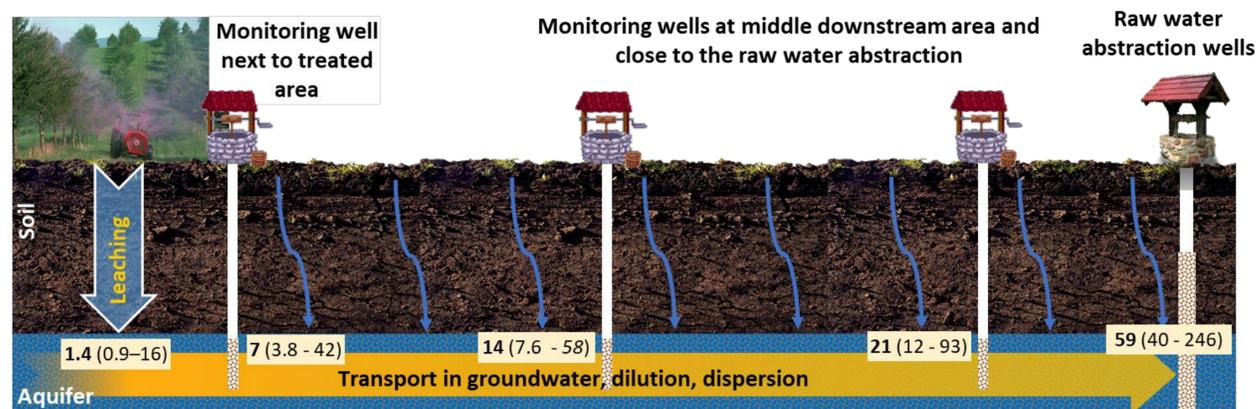
Results

As might be expected, the concentrations at each site, which were determined using both simulation and monitoring data, show a substantial decrease from the field to the abstraction well. A wide range of concentration gradients in sub-surface water was determined across the considered catchments. The final transfer factor from leachate at 1m depth to collected raw water is an approach to generate a heuristic "overall" factor of attenuation of pesticide concentration in sub-surface water.

A total transfer factor was calculated as the harmonic mean of the single gradients from each step at each catchment (Figure 1).

Table 1: Concentration of DMS in leachate and groundwater [µg/L], related gradients and transfer factor

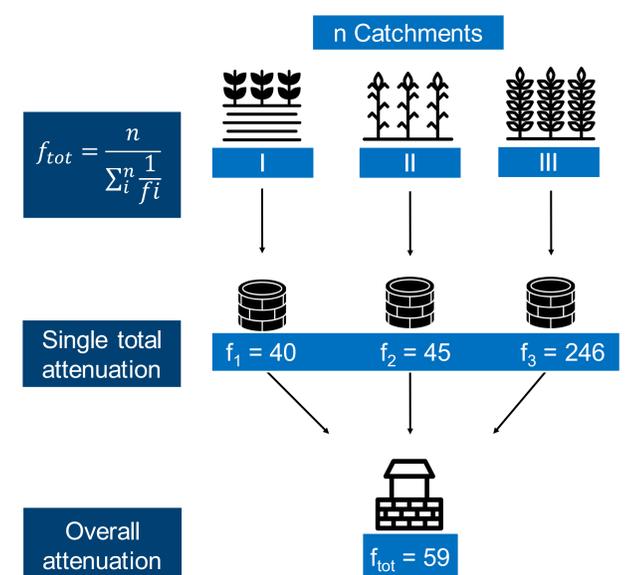| Attenuation Step	Catchment I	Catchment II	Catchment III	Range of gradients (cumulated)	Transfer factor (cumulated)
0 – FOCUS scenario Hamburg at 1 m depth	9.4	18	34		
1 – Leachate at 1 m depth	12	14	27		
2 – Leachate to aquifer	12	15 [a]	1.7	0.9 - 16	**1.4**
3 – Aquifer next to treated area	1.7	3.6	0.7	3.8 - 42	**7**
4 – Middle downstream area	0.7	1.8	*0.5* [b]	7.6 –*58*	**14**
5 – Close to raw water abstraction	0.6	1.1	0.3	12 - 93	**21**
6 – Collected raw water	0.3	0.3	0.1	40 - 246	**59**

[a] Following application, three consecutive years with very low annual precipitation resulted in excessive evapotranspiration leading in turn to a concentration and coelution of DMS from different seasons.

[b] value not available; interpolated mean of Step 3 & 5

$$f_{tot} = \frac{n}{\sum_i^n \frac{1}{fi}}$$

n Catchments

Single total attenuation: $f_1 = 40$, $f_2 = 45$, $f_3 = 246$

Overall attenuation: $f_{tot} = 59$

Figure 1: Scheme of a generalized overall transfer factor (f_{tot}) due to attenuation

As presented in Figure 2, the following observation points with increasing distance from the source area were considered:

- Shallow leachate in 1 m depth underneath treated area
- Bottom of the unsaturated zone, what represents the upper boundary of the aquifer
- Downstream monitoring well
  - Next to treated area
  - Middle downstream area
  - Close to raw water abstraction
- Raw water abstraction wells.

For the aim of modelling calibration, monitoring data from each step were compared with simulated DMS concentrations.

Monitoring well next to treated area

Monitoring wells at middle downstream area and close to the raw water abstraction

Raw water abstraction wells

Soil

Leaching

1.4 (0.9–16) 7 (3.8 - 42) 14 (7.6 - 58) 21 (12 - 93) 59 (40 - 246)

Aquifer

Transport in groundwater, dilution, dispersion

Figure 2: Harmonic mean of cumulative transfer factors from field to drinking water wells; range in brackets

Conclusions

Based on three case studies, an overall 59-fold attenuation of solute concentrations from shallow leachate to drinking water abstraction was observed.

These transfer factors can make a critical contribution to assess and support the interpretation of groundwater monitoring studies and to perform higher-tier exposure assessments.

Reference

Herrmann, M., Sur, R. Natural attenuation along subsurface flow paths based on modeling and monitoring of a pesticide metabolite from three case studies. Environ Sci Eur 33, 59 (2021). https://doi.org/10.1186/s12302-021-00490-2

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