Influence of Aquifer Parameters on Groundwater Residue Concentrations

Florian Hegler [1], Dirk Liss [2], Wenkui He [1], Olga Naeb [2], Stefan Reichenberger [1]
[1] Dr. Knoell Consult GmbH | Dynamostr. 19 | 68165 Mannheim | Germany | Contact: **fhegler@knoell.com** | **www.knoell.com**
[2] SGS Institut Fresenius GmbH | Im Maisel 44 | 65232 Taunusstein | Germany

Introduction

FOCUS leaching models are used in a regulatory context to calculate pesticide leaching flux concentrations at 1 m depth (PEC_{GW}; "Predicted Environmental Concentrations in groundwater"). These values are used in risk assessments in order to evaluate the impact of plant protection products on groundwater. In higher tier groundwater monitoring studies the properties of the saturated zone add additional complexity influencing actual pesticide residue concentrations in shallow groundwater. In this work the impact of groundwater flow velocity and aquifer porosity on groundwater residues for leachate concentrations from the unsaturated zone was determined. In this analysis using a realistic range of aquifer parameters the impact on the resulting residue concentrations in groundwater was quantified.

Methods and Scenarios

For the sensitivity analysis two representative sites were chosen each in Germany and Italy, which are characterized by a vulnerable soil profile and shallow groundwater depth. These sites are representative for regions in northern Germany and northern Italy. They have a similar soil profile but differ in their underlying aquifer characteristics in terms of grain size, porosity and hydraulic gradient. Residue concentrations in groundwater were simulated by coupling the leaching model FOCUS-PEARL (4.4.4) [1] with the open-source software OpenGeoSys [2]. A detailed description of the coupling methodology can be found in [5].

Germany: 2 fields of 1 ha each with the same soil profile in the unsaturated zone, but with different parameters for the underlying aquifer (one site with a high groundwater flow velocity and a second with a low velocity, cf. Table 1).
Italy: the same setup as in Germany, i.e. 2 fields of 1 ha each, one site with a high groundwater flow velocity and a second with a low velocity (cf. Table 1).
Weather time series for all four sites were obtained from the gridded weather dataset MARS 25 * 25 km² [3]. Extreme weather conditions in Italy in 2000 and 2006 led to regional flooding in North-Western Italy. For comparability reasons between the four sites, extreme weather conditions were replaced by average years.
Leaching simulations for the fields were carried out using FOCUS-PEARL with the respective field conditions and weather conditions with product applications on maize every fourth year at a rate of 1.5 kg/ha. Atrazine was selected as an active ingredient due to its low adsorption tendency (cf. Table 2). The leaching flux of atrazine was calculated in the PEARL simulations and was used as the upper boundary condition for the subsequent two-dimensional groundwater flow and solute transport simulations carried out using OpenGeoSys, in which resulting concentrations at a downstream monitoring well 1.5 m from the edge of the field were calculated. In order to be able to separate the influence of aquifer parameters from the influence of weather, in a second set of simulations the weather time series were swapped between the two sites of each country.

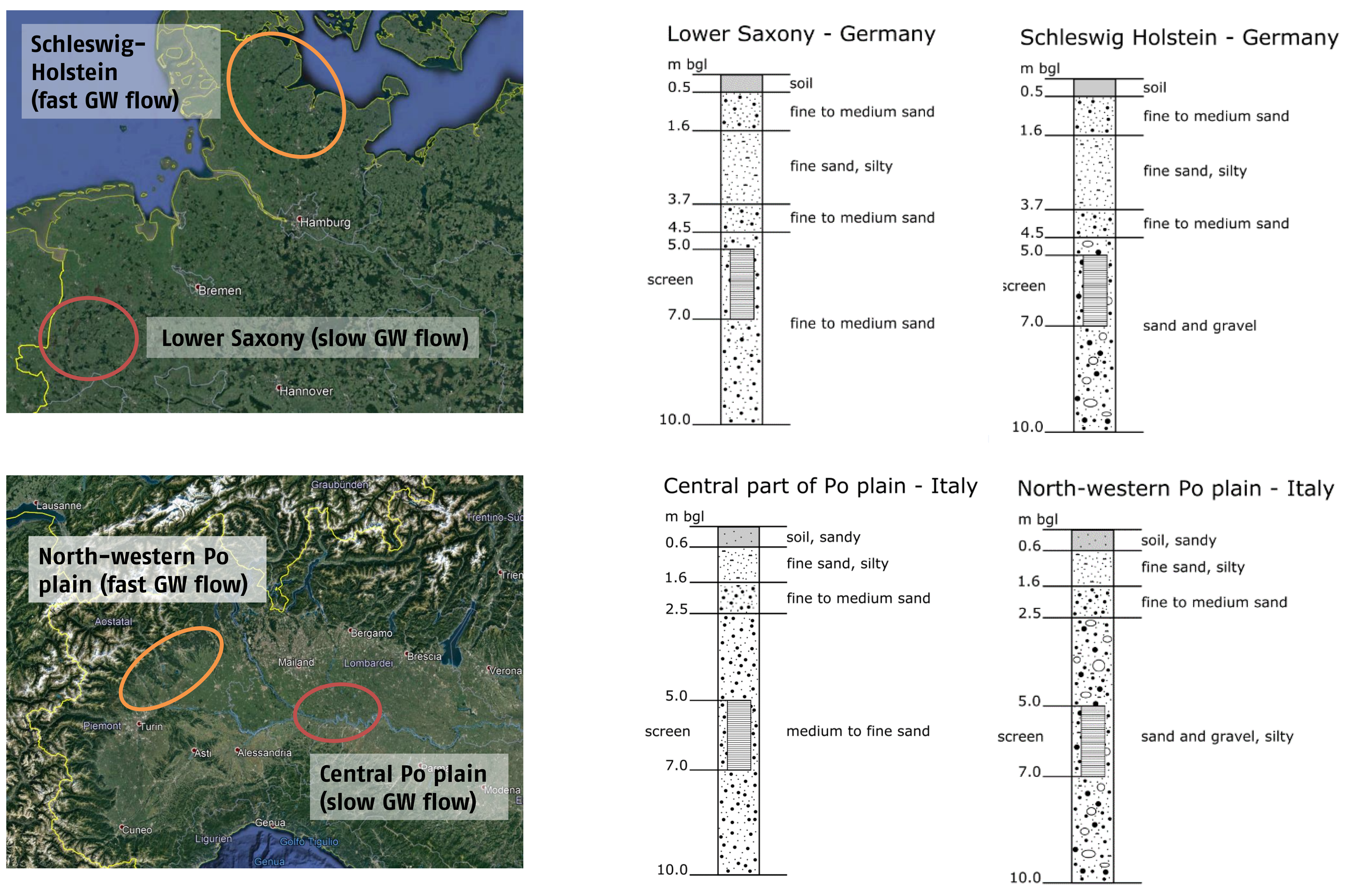

Figure 1: Location of target regions and representative soil profiles.

Table 1: Aquifer parameterization.

Location	Texture in aquifer	Characteristics	Long term annual average precipitation	Depth to GW	Hydraulic conductivity	Gradient	Porosity	GW flow velocity
	-		[mm/a]	[m]	[m/s]	[-]	[%]	[m/d]
Lower Saxony, DE	fine to medium sand	Fine grained, low gradient and flow velocity	772	5	1.0e-4	5.0e-4	12	0.036
Schleswig-Holstein, DE	sand and gravel	Coarse grained, high gradient and high flow velocity	726	5	7.0e-4	2.0e-3	18	0.672
Central Po plain, IT	medium and fine sand	Fine grained, low gradient and flow velocity	893	5	2.0e-4	8.0e-4	15	0.092
North-western Po plain, IT	sand and gravel, silty	Coarse grained, high gradient and high flow velocity	881	5	1.0e-3	4.0e-3	18	1.92

Table 2: Physico-chemical properties of Atrazine (based on the PPDB [4]).

Molar mass	Vapor pressure	Solubility in water	K_{foc}	Freundlich exponent	DT_{50} in Soil
[g/mol]	[Pa]	[mg/L]	[L/kg]	[-]	[d]
215.68	3.9e-5	35	174	1.07	66

Results and Conclusions

- The conclusions that can be drawn from the model simulations are applicable to both Italian and German scenarios.
- The local weather has a much larger influence (up to 200%) on modeled GW residue concentrations than the aquifer properties.
- A high groundwater flow velocity leads to a concentration time series with narrower and higher peaks. The lower flow velocity in the finer aquifer stratigraphy dampens residue peaks and increases the lag between application and peak concentrations.
- In the modeled scenarios, peak concentrations in fast flowing aquifers are typically around 20% increased.
- Even in fast flowing aquifers the modeled residue peak concentrations remain for several months and could influence the necessary sampling frequency in groundwater monitoring programs. However, the peak shape is based on the assumption that flow in the saturated and unsaturated zone is purely chromatographic without preferred pathways and fractures.

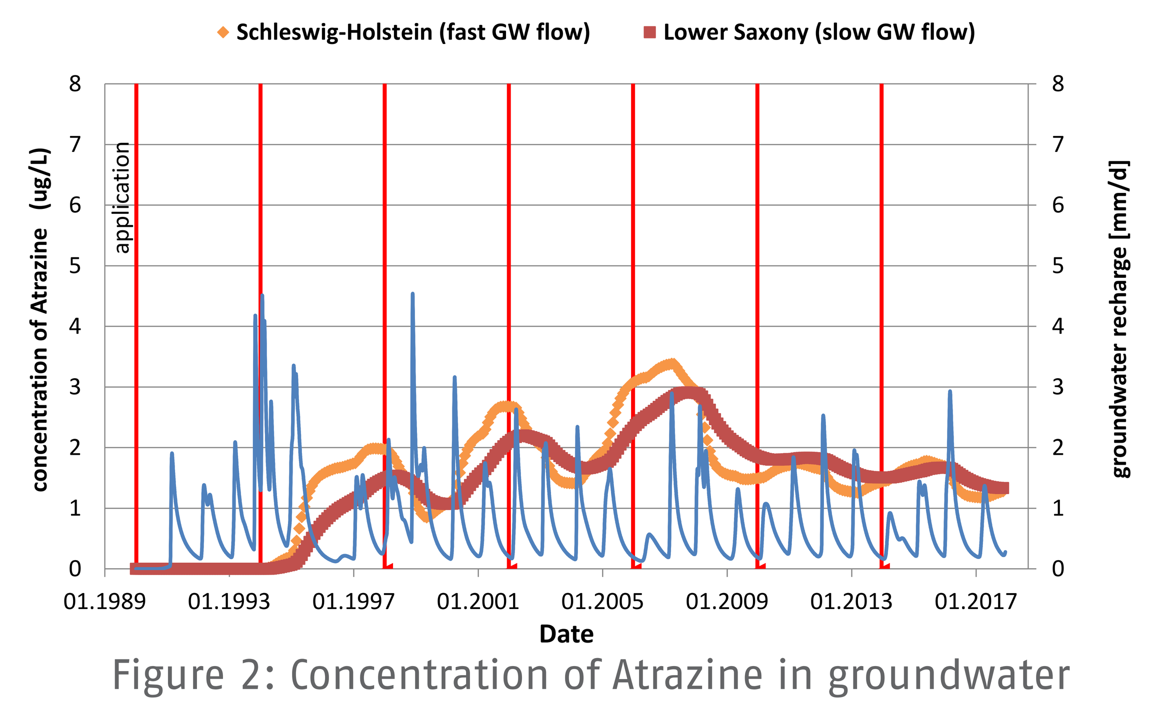

Figure 2: Concentration of Atrazine in groundwater modelled for both German sites with Lower Saxony weather data.

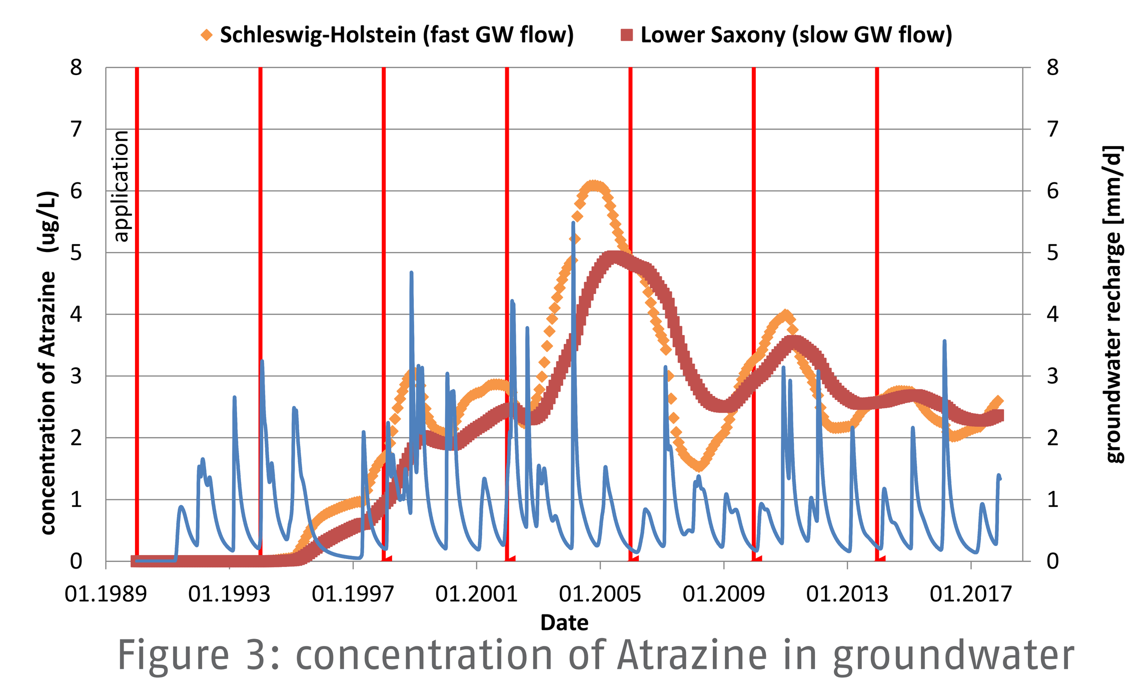

Figure 3: concentration of Atrazine in groundwater modelled for both German sites with Schleswig-Holstein weather data.

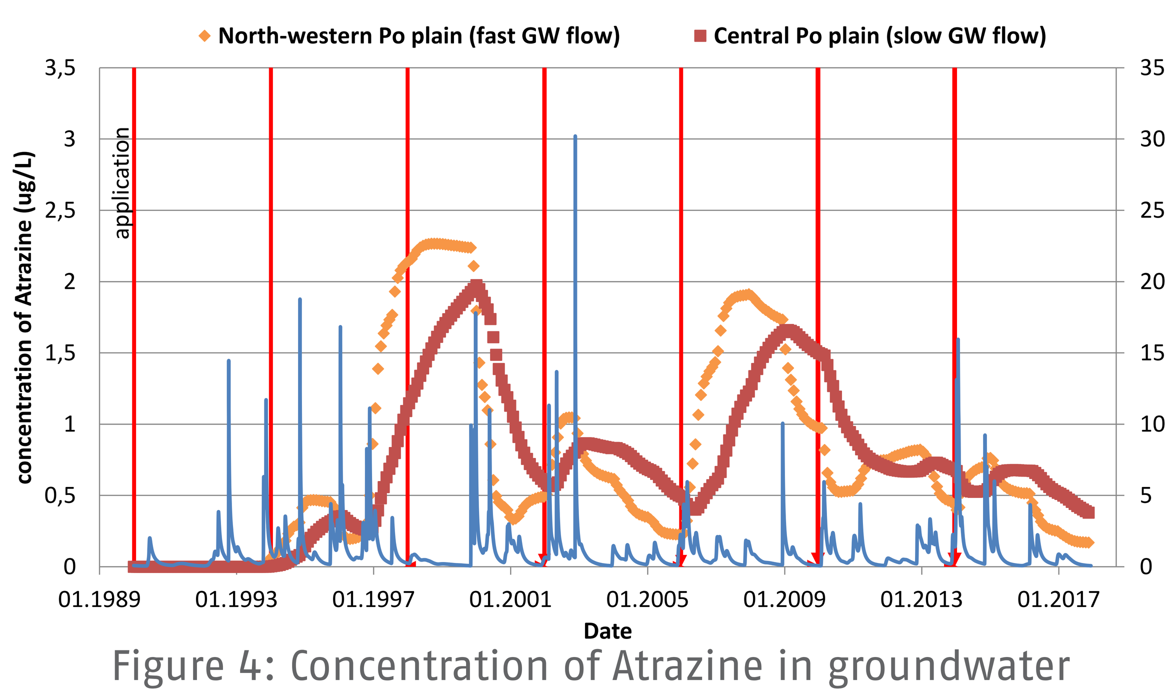

Figure 4: Concentration of Atrazine in groundwater modelled for both Italian sites with North-western Po plain weather data.

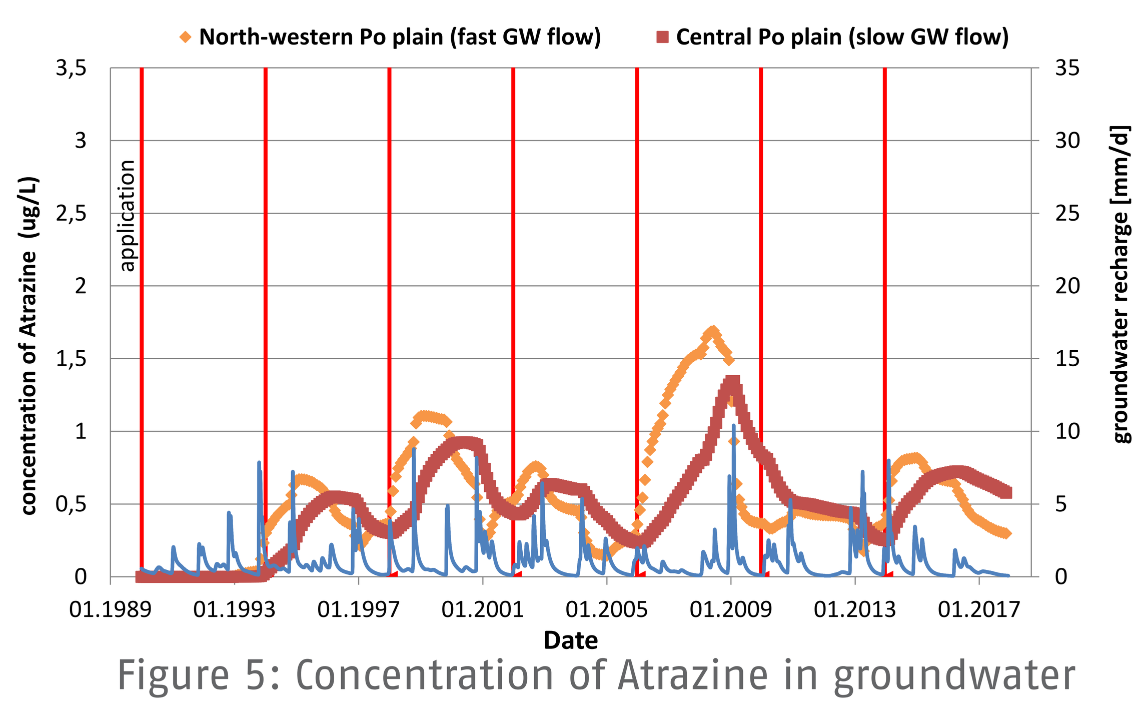

Figure 5: Concentration of Atrazine in groundwater modelled for both Italian sites with Central Po plain weather data.

References

[1] FOCUS (2014) "FOCUS groundwater scenarios in the EU review of active substances" Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev. 2, 202 pp.
[2] Kolditz, O., Bauer, S., Bilke, L., Böttcher, N., Delfs, J.O., Fischer, T., Görke, U.J.,Kalbacher, T., Kosakowski, G., McDermott, C.I., Park, C.H., Radu, F., Rink, K., Shao, H., Shao, H.B., Sun, F., Sun, Y.Y., Singh, A.K., Taron, J., Walther, M., Wang, W., Watanabe, N., Wu, Y., Xie, M., Xu, W., Zehner, B. (2012): OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media, Environ. Earth Sci.
[3] MARS-AGRI4CAST (2016): Gridded Agro-Meteorological Data in Europe. European Commission – Joint Research Center, 1975–2016, version 2.0.
[4] Lewis, K.A., Tzilivakis, J., Warner, D. and Green, A. (2016): An international database for pesticide risk assessments and management. Human and Ecological Risk Assessment: An International Journal, 22(4): 1050 - 1064. DOI: 10.1080/10807039.2015.1133242.
[5] He, W., Miles, B., Staudenmaier, H. (2017): A generic modeling exercise to identifying factors influencing the representativity of measured pesticide concentrations at groundwater monitoring wells, International Conference on Pesticide Behaviour in Soils, Water and Air, University of York.