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REXPO: A catchment model designed to understand and simulate the loss dynamics of plant protection products and biocides from agricultural and urban areas

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SUMMARY

During rain events, biocides and plant protection products are transported from agricultural fields but also from urban sources to surface waters. Originally designed to be biologically active, these compounds may harm organisms in aquatic ecosystems. Although several models allow either urban or agricultural storm events to be predicted, only few combine these two sources, and none of them include biocide losses from building envelopes. This study therefore aims to develop a model designed to predict water and substance flows from urban and agricultural sources to surface waters. We developed a model based on physical principles for water percolation and substance flow including micro- (also called matrix-) and macropore-flows for the agricultural areas together with a model representing sources, sewer systems and a wastewater treatment plant for urban areas. In a second step, the combined model was applied to a catchment where an extensive field study had been conducted. The modelled and measured discharge and compound results corresponded reasonably well in terms of quantity and dynamics. The total cumulative discharge was only slightly lower than the total measured discharge (factor 0.94). The total modelled losses of the agriculturally used herbicide atrazine were slightly lower (∼25%) than the measured losses when the soil pore water distribution coefficient (describing the partition between soil particles and pore water) (K_d) was kept constant and slightly higher if it was increased with time. The modelled urban losses of diuron from facades were within a factor of three with respect to the measured values. The results highlighted the change in importance of the flow components during a rain event from urban sources during the most intensive rain period towards agricultural ones over a prolonged time period. Applications to two other catchments, one neighbouring and one on another continent showed that the model can be applied using site specific data for land use, pesticide application, weather and literature data for soil related parameters such as saturated water content, hydraulic conductivity or lateral distances of the drainage pipes without any further calibration of parameters. This is a promising basis for using the model in a wide range of catchments.

1. Introduction

Plant protection products are detected in surface waters mainly during the application period, and biocides, throughout the year (Squillace and Thurman, 1992; Kreuger, 1998; Hoffmann et al., 2000; Gerecke et al., 2002; Neumann et al., 2002; Wittmer et al., 2011a; Moschet et al., 2014). Originally designed and used to control unwanted organisms in agricultural and urban environments, these compounds are washed off during storm events and can affect non-target organisms and entire ecosystems once lost to the aquatic environment (Liess and Schulz, 1999; Cuppen et al., 2000; Chèvre et al., 2006; Ashauer et al., 2011).

For a long time, agriculture has been regarded as the main source of surface water pollution with biocidal products. Only more recently have urban losses received more attention. First

Abbreviations: K_d, distribution coefficient; CSO, combined sewer overflow; CS, combined sewer; SS, separate sewer; WWTP, wastewater treatment plant.

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studies on losses from building envelopes (such as roofs and facades, e.g. Bucheli et al., 1998; Burkhardt et al., 2009) as well as on losses due to plant protection product applications by private gardeners or municipal services (e.g. Wittmer et al., 2011a; Ramwell et al., 2002; Blanchoud et al., 2007) showed that the urban contribution can be substantial. This raised the question as to whether agriculture is in fact the main source here, or whether more attention should be paid to the urban losses of biocidal compounds (Hoffmann et al., 2000; Jongbloed et al., 2004; Skark et al., 2004; Blanchoud et al., 2007; Woudneh et al., 2009).

The dynamics of urban and agricultural losses in surface waters can be analysed by sampling surface waters during rain events (Wittmer et al., 2010; Wittmer et al., 2011a). However, to separate the various processes leading to the observed load and discharge dynamics in a comprehensive and consistent way requires a modelling approach. In order to simultaneously assess the importance of the various sources and input pathways as well as to simulate the effect of different mitigation measures, a model is required which can represent both urban and agricultural sources. In fact, most European catchments show mixed urban and agricultural land use. In humid climates, such as Switzerland, most plant protection product and biocide losses to surface waters are driven by rainfall. Thus, the model should simulate all relevant storm water flows (e.g. preferential flows to drains, combined sewer overflows (CSO)) as well as substance mobilization and transport from the source (e.g. biocides from facades).

Many studies have shown that the transport of agrochemicals (plant protection products, veterinary antibiotics) and phosphorus from agricultural fields is mainly due to fast flow processes, such as surface runoff, erosion or preferential flows to tile drains (among many others Beven and Germann, 1982; Klavidko et al., 1991; Stamm et al., 1998; Kohler et al., 2003; Stoob et al., 2005; Doppler et al., 2012). These flow processes are a function of rain intensity, duration and very importantly also of the antecedent saturation conditions of the soils. Water flows in soil show a strongly non-linear behaviour and are characterized by flows through porous media only partially saturated by water (Brooks and Corey, 1966; Mualem, 1976; Schiffler, 1992). Several models exist which take both unsaturated and saturated flows in the soil matrix into account and add an additional compartment for preferential flows through macropores (known as dual porosity models). For a comprehensive review see Köhne et al., 2009). Commonly used models include MACRO (Larsbo and Jarvis, 2003) and HYDRUS (Simunek et al., 1999). Both of them are widely used for soil columns or on a field scale to predict both water and substance flows. Only few models exist on a catchment-scale of several square kilometers (Köhne et al., 2009). Freeze and Harlan (1969) already concluded that catchment-based models require a physically sound integration of the processes in the surface zone, the unsaturated zone as well as the groundwater zone. This was also emphasized by Köhne et al. (2009). Borah and Bera (2003) presented a review of the mathematical principles of currently available catchment-scale models. Most of these models focus only on agriculture; the only one dealing with urban and agricultural areas was HSPF (Bicknell et al., 1997). However, to our knowledge HSPF is not based on a dual-porosity approach. Further limitations of the reviewed models were that many of them are designed for long-term simulations and thus only provide daily time steps, a procedure which is unsuitable for the analysis of storm events (e.g. SWAT Neitsch et al., 2005). A further aspect is whether catchment models necessarily have to be spatially explicit (which requires large data inputs) or whether approaches using spatially lumped sources can represent the most important processes. The findings of a model comparison by Reed et al. (2004) suggest the latter to be often the case.

One way of getting round the lack of combined urban and agricultural models would be to couple two single models. However, most commercially available urban models focus either on the urban drainage system (e.g. SIMBA®sewer (Erbe et al., 2002)), or the sewer model by Mannina and Viviani, 2010) or the WWTP (e.g. STOAT, SIMBA®: Erbe et al., 2002; Rauch et al., 2002) and only few represent the entire system from sources to surface waters. They are often a combination of different programs (Erbe et al., 2002). A reason for this lack of integrated catchment models might be that urban models are usually intended for engineering purposes, such as the design and sizing of drainage system components for flood control. Programs which do include various urban aspects include SWMM (James et al., 2003) and CITYdrain (Achleitner et al., 2007). SWMM also has an unsaturated soil module, but does not include preferential flows to drains. Both models deal with conventional urban stormwater pollutants such as suspended solids and continuous pollutants from households. Both models use an input function for household pollutants and a build-up rate after storm events for suspended solids. However, biocides in facades, for example, show a different wash-off and stock behaviour than solids on streets (e.g. Schoknecht et al., 2003; Burkhardt et al., 2009). In a previous study therefore, we developed a model to simulate the wash-off from outdoor construction materials.

Although several models cover single aspects of plant protection product and biocide losses from urban and agricultural areas, none of them can represent both land use types adequately. Several models would have to be coupled in order to cover all sources and input pathways. However, coupling of various models requires them to be on the same level of complexity (e.g. one-dimensional to three-dimensional) and to provide the same time steps. We consequently developed a new model, henceforth called REXPO, to simultaneously simulate realistic exposure scenarios of plant protection products and biocides from urban and agricultural areas. The aim was to keep the model structure relatively simple, as suggested by Branger et al. (2009). The requirements are:

1. The model represents both urban and agricultural sources and all relevant storm-water flows.
2. The model adequately represents the mobilization of compounds at the source.
3. The model is able to represent the most important hydrological processes in soils, including processes at the surface, in the unsaturated zone and in the saturated zone.
4. The model is applicable to a catchment of several square kilometres without extensive parameterization.
5. The time steps of the model can be chosen by the user in order to adequately represent storm events.
6. The model concept is based on physical principles and all the parameters used have a physical meaning.
7. The model shall be as simple as possible but complex enough to simulate the observed patterns of discharge and compound concentration.

The presented model is applied to a catchment in which we had previously conducted a an intensive field study. The catchment consists of various degrees of urban and agricultural land use (Wittmer et al., 2010). We will address the following questions:

1. Which key sources influence (a) the peak loads of plant protection products and biocides to surface waters and (b) the cumulative loads to surface waters?
2. Which are the most relevant entry paths for the compounds?
3. Which are the key parameters driving the inputs to surface waters?
4. Which knowledge gaps are limiting our modelled results?