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Quantification of water flow and transport in soils

Christine Stumpp[1*]

Zusammenfassung

Lysimeter eignen sich Wasser- und Massenflüsse in der ungesättigten Zone zu untersuchen. Durch den Einsatz von Umwelttracern oder künstlicher Tracer können zusätzliche Informationen generiert werden, so dass diese Tracer zu einem verbesserten Prozessverständnis von Wasserflüssen und Stofftransport beitragen. Zusammen mit der mathematischen Modellierung lassen sich somit unter anderem die Verweilzeiten des Wassers, bodenhydraulische Eigenschaften oder spezifische Transportprozesse identifizieren und quantifizieren. Es wird auf mehrere Beispiele eingegangen, in denen Tracer zusätzlich zum Monitoring eher klassischer Variablen (Wassergehalt, Matrixpotential, Sickerwassermengen) herangezogen wurden, um somit Fließ- und Transportprozesse in der ungesättigten Zone noch besser verstehen und quantifizieren zu können. Diese Beispiele beinhalten die Bestimmung von Verweilzeiten in unterschiedlichen Böden und bei unterschiedlicher Landnutzung, die Untersuchung von Fließheterogenität in Lysimeterreplikaten und die verbesserte inverse Modellierung zur Quantifizierung von bodenhydraulischen Eigenschaften und Transportparametern. Des Weiteren werden Möglichkeiten aufgezeigt, bei denen der Einsatz von Umwelttracern für zukünftige Fragestellungen herangezogen werden könnte, um offene Fragen in der Bodenhydrologie und in der Ökohydrologie zu beantworten.

Schlagwörter: Lysimeter, Tracer, stabile Wasserisotope, mathematische Modellierung

Summary

Lysimeters are perfect tools to investigate water and mass fluxes in the unsaturated zone. Using environmental or artificial tracers in these experimental setups can further advance our understanding of flow and transport processes. In combination with mathematical models water transit times, hydraulic properties or specific transport processes can be identified and quantified. Here, several examples are presented on how tracers can be used to gain additional information about water flow and transport in the unsaturated zone compared to more traditional soil hydrological monitoring approaches. These examples include the estimation of water transit times for different soils and different land use, the identification of flow heterogeneities in lysimeter replicates, and inverse modelling approaches for quantification of soil hydraulic properties and transport parameters. Further, current challenges and future opportunities in combining tracer approaches and lysimeter experiments are presented for solving open research questions in soil hydrology.

Keywords: lysimeter, tracer, water stable isotopes, mathematical modelling

Introduction

Importance of Lysimeters

Lysimeters are perfect tools to investigate water and mass fluxes in the unsaturated zone. Processes can be studied in a definite soil volume. Despite high costs, the advantages of lysimeters are the controlled and measurable boundary conditions enabling mass balance calculations for both, water and solutes. They can be seen as an intermediate experimental setup between laboratory soil columns and field studies. There are many different setups ranging from very simple boxes to high precision lysimeters (Pütz et al. 2016). Recent technical developments and research is summarized in Pütz et al. (2018) highlighting that lysimeter studies have been used to investigate evaporation, evapotranspiration, recharge, and leaching as well as improve modelling.

Importance of Tracers

Artificial tracers are applied in the hydrological cycle to get information about water flow and transport (Leibundgut et al. 2009). In lysimeters, conservative tracers are often combined with reactive contaminants (as tracers) allowing to understand the fate of these contaminants (e.g. pesticides) in the unsaturated zone and to quantify leaching (Schuhmann et al. 2016, Torrentó et al. 2018). Most commonly used artificial tracers are salts and dyes (Flury & Wai 2003, Leibundgut et al. 2009). For example, bromide and deuterated water were used as artificial tracers to identify different flow components and to quantify flow and transport parameters

[1] Institut für Hydraulik und landeskulturelle Wasserwirtschaft, Universität für Bodenkultur Wien, Muthgasse 18, A-1190 WIEN
[*] Ansprechpartner: Univ. Prof. Dr. Christine Stumpp, christine.stumpp@boku.ac.at

by comparing different modelling approaches (Stumpp et al. 2009b). Generally, the gained information from artificial tracer experiments performed for a specific time period strongly depends on the initial (soil water content) and boundary conditions (infiltration, precipitation, evapotranspiration) during this specific time period. Thus, results are only valid for these specific conditions and might not be representative for the system at other times (Leibundgut et al. 2009). In turn, it enables to study specific processes under specific initial and boundary conditions, like the initiation and quantification of preferential flow (Allaire et al. 2009).

In contrast to artificial tracers, environmental tracers are beneficial when covering processes at larger scales and/or over long-time periods. They provide integrative information about both water flow and transport. Environmental tracers are substances already present in the environment and provided by nature (e.g. stable and some radioactive isotopes, temperature, chloride) or anthropogenic input (like tritium or noble gases). For studying water flow and solute transport, the hydrogen and oxygen isotopes are of special interest. As being part of the water molecule, $\delta^{18}O$ and $\delta^{2}H$ provide a tracer signal with every precipitation event over a certain space. Due to fractionation effects, stable isotopes of water have a seasonal distribution in precipitation with more depleted values in winter (colder season) and more enriched values in summer (warmer season) (Clark & Fritz 1997). Following the seasonal distribution of stable isotopes in the soil water, and its relative changes since that water fell as snow or rain, gives integrative information not only about water flow but also about transport processes with time and depth below ground. The seasonal distribution is attenuated due to dispersion and thus enables to study flow in systems with transit times about ≤ 5 years - depending on the dispersivity of the system.

Flow and transport

Mathematical Modelling

Lumped parameter modeling is a less parameter-intensive method compared to the traditional numerical modeling approaches used for studying flow and transport processes. It was shown in lysimeter experiments with bare, sandy soils using environmental isotopes as tracers that this modelling approach gives adequate results even in the unsaturated zone and is comparable to numerical modeling of water flow and tracer transport (Maciejewski et al. 2006, Maloszewski et al. 2006). However, the application of the lumped parameter model for agricultural soils is challenged by strongly variable water flux during crop periods (Stumpp et al. 2009a). One of the most important challenges in applying the lumped parameter approach is the estimation of the tracer concentrations in the recharging water (input function) based on the available data. Several methods (e.g. calculating seasonal recharge factors) were developed for the application under saturated conditions and at catchment scale (McGuire & McDonnell 2006). For soils, a method was developed to estimate the isotope input function of recharging water (Stumpp et al. 2009c). The new input function was based on the actual evapotranspiration rates which were determined indirectly from the change in mass of the lysimeter. Thus, only precipitation events were considered effectively contributing to the lysimeter discharge. The combination of the new modified input function and splitting the observation periods into individual vegetation periods greatly improved the lumped parameter model outputs compared to the unmodified input data. The reliability of the lumped parameter model was confirmed by comparing the fitted and measured values, and the parameters to those derived from numerical modeling with HYDRUS-1D which is state of the art for transient water flow and transport modeling (Šimůnek et al. 2008). Both model approaches resulted in similar dispersivities and mean water contents, which were also in the same range as the measured values.

When simulating the transport of water stable isotopes, fractionation processes need to be considered and isotopes cannot be treated like other solutes at the upper boundary. If fractionation processes can be neglected though, a modified version of HYDRUS-1D can be used to account for isotope transport (Stumpp et al. 2012). Here, the relative concentration of isotopes (delta content) does not accumulate at the upper boundary due to evaporation. This is in contrast to the standard treatment of solutes during evaporation in HYDRUS-1D, where solutes stay behind in the soil while water is removed. This modified version has been used not only for the simulation of water flow and transport in lysimeters (Groh et al. 2018) but also for the interpretation of isotope data from soil cores (Sprenger et al. 2016).

For calibration of numerical water flow and transport models and for the inverse estimation of soil hydraulic properties usually water content and/or matric potential measurements are used. However, no direct information on transport can be gained from these data. We showed that water stable isotope data contained additional information and significantly improved the inverse estimation of soil hydraulic and of transport parameters (Groh et al. 2018). Here, a combined integration of water content, matric potential and isotope data in one objective functions gave better results compared to a sequential optimization procedure.

Land use effects

Land cover and agricultural management practices can significantly influence soil hydraulic properties, bulk density, and soil structure. In lysimeter experiments, it was investigated whether these changes near the soil surface, resulting from different fertilizer applications or land cover, have any net effect on water transit times and groundwater recharge over long time periods or whether they merely impact soil structure. Five lysimeters containing undisturbed soil monoliths from the same agricultural field site were investigated over a period of five years in Gumpenstein (Stumpp et al. 2012). Liquid cattle slurry and solid animal manure were applied to the lysimeters containing soil planted with maize and winter rye. The lysimeters that had a cover of grass/clover were treated with mineral fertilizer. The influence of land cover and type of fertilizer application on water flow and solute transport was quantified for all lysimeters using a modified version of HYDRUS-1D. The highest drainage was observed in the maize lysimeter treated with cattle slurry, and the lowest in the grass lysimeter treated with mineral fertilizer. Pronounced differences in water contents and estimated saturated hydraulic conductivities between the lysimeters were restricted to the upper 25 to 30 cm of the soil. In particular, the lysimeters treated with animal manure had higher porosities, indicating a higher content of organic matter. Main differences in discharge between the lysimeters were observed in spring and during the plant growth periods, indicating the importance of non-uniform, patchy infiltration patterns during snow melt and of root water uptake, respectively. Mean water flow velocities, transit times and effective water contents were estimated from the stable water isotope data, providing evidence of the impact of land cover and type of fertilizer application. Smaller mean transit times were found in the maize lysimeters and for soils with liquid cattle slurry applications. Simulations indicate that numerical modeling can reproduce the general trend of water flow and isotope transport. Despite differences in mean transit times, fitted dispersivities were all in the same range, suggesting similar soil structures in the five lysimeters. However, more data for calibration and more information about heterogeneous infiltration would be required to improve the model accuracy. In general, stable water isotopes clearly added value, elucidating differences in mean flow parameters between the lysimeters. Thus, they provided evidence of the impacts of land cover and fertilizer applications, which are not obvious from water balance and mean discharge rates alone.

Outlook

Measuring hydrogen and oxygen isotope ratios in soil pore water or in the drainage of lysimeters have certainly advanced our understanding of water flow and transport processes in the unsaturated zone. There are many other opportunities where the combined use of lysimeters and tracers can help to better understand the dynamic interplay of hydrological, geochemical and ecological processes (Stumpp et al. 2018). For the application of water stable isotopes, this includes processes like snow melt infiltration, evaporation or the separation of transpiration and evaporation. For examples, it could be answered in which depths plants take up water and how long this water has been stored in the unsaturated zone. In addition, new automated systems that can provide high-resolution in-situ measurements and real-time data analysis have now been developed. These technological breakthroughs are thus poised to improve our understanding and the modeling of water and matter fluxes in the atmosphere–plant–soil–groundwater continuum.

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