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Interactive comment on "Mass transfer effects in 2-D dual-permeability modeling of field preferential bromide leaching with drain effluent" *by* H. H. Gerke et al.

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We thank the three referees for their helpful and constructive comments that will contribute to improve this dual-permeability based analysis of preferential flow in structured soil. Referee #1 raised a number of additional questions (i.e., what about mass transfer effects in sandy drained soils, in non-drained soils, or effects of spatial heterogeneity and macropore wall coatings) that can help directing future analysis. First of all, we apologize for lack in clarity that led to a number of misunderstandings. It seems that we failed to present the focus and the differences between old and new aspects and

between general and specific conditions clear enough. We appreciate all suggestions related to the writing style and figure formatting. This relatively complex analysis relies heavily on previously published work. It is obviously not easy to define the level of comprehensiveness necessary for understanding this study as reviewer comments indicate. Referee #1 wants to see a clear separation between old and new work, referee # 2 seems to require more information and additional work, and referee #3 suggests carrying out a larger sensitivity analysis and considering equifinality. Major parts of the concerns of the referees are related to aspects that were already discussed in previous papers (Gerke and Köhne, 2004; Köhne and Gerke, 2005; Gerke et al. 2007; Dusek et al. 2008) including, for instance, scenarios where Br enters the soil through the PF domain or sensitivity to values of the exchange coefficient αws. In the revised manuscript we will make sure that it is always clear what is new and what is already included in the previous studies. The focus of the analysis is to improve our understanding of local effects between-domain mass transfer in the dual-permeability model of a vertical cross-section and how it affects the overall solute response at the field-scale. At this stage, we did not intend to carry out a full sensitivity or uncertainty analysis or to optimize the model parameters. With the help of these scenarios, we wanted to better understand the model, as a step before starting more detailed analyses owing to the complexity. We think that the experimental conditions are well-suited for analyzing effects across the scales from mass exchange coefficients, representing local-scale soil structural properties, to plot and drain discharge and bromide effluent, representing the integrated field-scale signals. Intention is to explain the assumed upscaling effect with one possible model approach; the comparison with data is to show that this approach is not completely unrealistic. The limitation of the present analysis on the diffusive exchange component and on the upper solute boundary restriction (i.e., that bromide exclusively enters the soil matrix (SM) domain) resulted from previous studies. This restriction allows a more detailed analysis of the mass transfer effects in the 2D modeling procedure and a better explanation of the complexity of the simulation results across the scales. The various aspects of the complex system (i.e., dual-permeability modeling, comparing 1D and 2D approaches, aspects on model parameter calibration and sensitivity analysis and the scale issues) requires a somewhat larger review part. In the revised version, we will try to present the ideas in a more concise but still detailed form.

Here, we can reply to the major comments as follows:

A) The assumption that bromide is entering the soil surface only through the soil matrix domain is a result of previous work based on a number of simulation tests, and was extensively discussed in Gerke et al. (2007). Solute influx in both domains resulted in a large over prediction of bromide leaching. In conclusion of that work (and other simulations in which the water transfer coefficients were tested), we found that a higher concentration peak at the second day of irrigation could be reproduced only when assuming that bromide enters through the SM domain. This assumption could possibly be realistic; however, in the field it will never be as drastic as it is possible to describe in the simulation. We noticed that especially these effects of the solute boundary conditions (BC) provide a novelty and are great challenge for future observations and analyses of solute movement in structured soil. We agree, of course, that the sensitivity of the mass transfer coefficient is affected by the initial mass distribution, and also by the boundary fluxes. We could easily add another scenario with bromide influx in both domains and show that the sensitivity of the exchange coefficient αss is high as well; however, there is no match with data (c.f., Fig. 7 of Gerke et al., 2007). Also, we already assumed bromide influx in form of resident as well as flux BC in the preferential flow domain (Dusek et al., 2008), which resulted in serious overestimation of Br mass effluent. Here, we wanted to focus only on scenarios already known to be close to data. However, we admit that our sensitivity study of mass transfer parameter is dependent on specific experimental conditions at the Bokhorst site. The focus on the diffusive mass transfer component allowed us to more intensively study the dual-permeability model response as function of irrigation and rain conditions. Such comparative analysis of effects of the solute mass transfer coefficient αss requires the water transfer to be identical. Also, as

previously studied, the water transfer coefficient αws was found less sensitive for the present conditions.

B) The main innovation (referee #1) is to trace back the leaching at the outlet of the subsurface-drained field to local effects of mass transfer interacting with soil surface boundary conditions. Novel is also the analysis of the solute inter-domain exchange for plot-scale irrigation with ponding as compared to the rain acting on the field-scale. Furthermore, the interplay between water and solute transfer in the 2D flow domain provides novel insights in interpretation of spatial and temporal distributions of effluent and residual tracer concentrations. The main message (referee #1) of this paper is that small-scale local properties cannot be neglected – at least for the conditions assumed here. The effects of local properties remain sensitive even if fluxes on the catchment scale are considered. In addition, the results suggest a more careful consideration of initial conditions (i.e., distribution of solutes between domains) and boundary conditions (i.e., domain-specific infiltration rates) in structured soil. For a better quantification of preferential flow, more complex experiments should be designed such as to consider the domain-specific conditions. The results demonstrate that amount and composition of the drain effluent in the model framework depend on a complex interrelation between temporally and spatially variable mass transfer in the 2D vertical flow domain. Mass transfer is a result of varying contributions of advective and diffusive components, of spatial distributions of residual tracer concentrations, and of lateral flow fields in both domains at all plots of the subsurface drained field.

C) Equifinality (Referee #3) is of course a problem. However, it was not our intention to deal with finding “the optimal” parameter combination nor did we focus on analyzing such issue. We wanted to work with possible scenarios in order to get better insights in the dual-permeability model and its effects across scales on the catchment scale as an example. Here, with the few remaining parameters that are not limited by experimental data ranges, it may be difficult to find parameter combinations that simultaneously allow describing drain discharge and effluent concentration as well as the soil water matrix potentials and the residual bromide distribution in the soil similarly well. We did not intend to fit the model to data. This would lead to a separate study with a detailed uncertainty analysis (beyond the scope of the present study). Our focus is rather to demonstrate (probably for the first time with such a modeling approach) how local-scale properties may affect processes at the larger scale. The study is pointing to open problems when dealing with preferential flow modeling. We have also not included many other aspects (e.g., spatial heterogeneity) and showed only one possible description of flow and transport in the system. Our intention was to explain the dual-permeability model behavior in greater detail and to point out to challenges in experimentation and modeling.

D) The 1D-2D effects (Referee #1) have been analyzed and discussed previously for this experiment (Gerke et al., 2007): Yes in the 1D simulation all the heterogeneity and lateral transport components are included in the effective parameters of the coupled models limiting the physical basis and explanations. The 2D simulations include most important physical aspect such as the lateral soil water and solute movement towards a drain. Soil heterogeneity is not included yet. The 3D case would add more information only if flow paths strongly deviate from the cross-section concept. Within our focus (i.e., analysis of local effects of mass transfer on larger scale plot and field scale Br-leaching), the 1D approach recalls the motivation, and differences between 1D and 2D approach are reviewed to explain the more complex 2D system.

E) Mass flux versus concentrations: We note that the measurement of bromide concentrations is based on mixed water samples taken by automated sampler providing aliquots of drain discharge water over a period of time. This means that concentration data are not fully independent of fluxes. We calculated the Nash-Sutcliffe (NS) coefficients based on the concentrations (no parameters were calibrated in this study); we always look on the water drainage curve and bromide concentration curve. We can easily provide the values of the coefficient of determination (i.e., values range between 0.56 and 0.78), which are consistent with NS values. Since the predicted drainage

rates are slightly overestimated and bromide concentrations underestimated, the resulting predicted Br mass fluxes accidentally mimic the measured flux. Nevertheless, the overestimation of drain discharge is relatively small (Fig. 4); base flow is slightly overestimated (c.f., Figs. 3 and 11 in Gerke et al., 2007) during the period before irrigation.

F) Advective versus diffusive mass transfer (Fig. 11): Referee # 2 believes that a change in values of the water transfer coefficient αws (which is assumed constant here) would determine very different response of the model because advective mass transfer is the dominant component. This appears logical; however, we previous simulations based on different values of αws did not match at all. The relatively small values of αws were selected before. Larger αws value would lead to increasing local equilibrium conditions in pressure heads and less preferential flow. We will include a note on this in the revised version. Still advective transfer component acts in addition to the diffusive transfer because the domain-specific concentrations are affected by advective transfer of bromide.

G) Additional aspects: Referee # 1 has raised a number of interesting questions that cannot sufficiently be discussed in the present study:

(i) A discussion on the importance of transfer term parameter in sandy drained soils would be interesting but beyond the scope here. This dual-permeability approach is for structured soil; finer-textured soils are differently-structured than coarse-textured soils. Drained sandy soils are completely different systems with other types of structure and preferential flow mechanisms. If the sandy soil is wettable, large mass transfer provides local equilibrium conditions. Preferential flow on sandy soil is frequently induced by water repellency and described with different approaches (e.g., de Rooij, 2000).

(ii) For non-drained fields with groundwater flow to the nearest ditch or brook, preferential flow can possibly be important also when drainage elements are far apart; the same 2D model will be limited as for hillslope systems, by the relation between (relatively large) length and (relatively small) depth. Here drain spacing and non-drained soils were not tested. Nevertheless, the same model could be used if structured soils are present. The response times could be larger but the effects would be similar. (iii) Water table heterogeneity in the field could affect upscaling flow from a 2D cross-section to the entire field by variation in the weighing procedure. It is not clear if it can be neglected. We expect that the spatial heterogeneity of the preferential flow domain is the most sensitive part. Since we have seen strong effects of the surface boundary conditions, the heterogeneity in combination with local exchange is probably important. This is not studied yet.

(iv) Wall coatings of preferential flow paths can be highly effective. Coating effects are imitated here by reduced values of the water and solute mass transfer coefficients αws and αss, respectively; "reduced" means that the values are smaller as those of comparable soil matrix properties (i.e. the effective exchange term hydraulic conductivity and diffusion coefficients in the original formulation (e.g., Gerke and Köhne, 2004) are the same as those of the soil matrix domain). The effect of coatings on the water exchange has already been included and was analyzed before; the current values are reduced as compared to those of the soil matrix domain.

(v) Fig. 4: We note that simulation results separately for the preferential flow and the soil matrix domains are not possible at the field scale. This is simply due to the upscaling and weighing procedure for calculating field scale simulation results. The impression that the quality of the fit depends on the soil moisture conditions is misleading, because the soil is highly water saturated throughout the specific period of interest. We rather think that information is missing that could clarify the over prediction of discharge and thus the larger cumulative mass flow during the second irrigation day. Test with different values of the water transfer coefficient αws did not clarify this problem.

(vi) Bromide infiltration during redistribution of ponding water at the end of the first irrigation period (referee # 2) is not considered (Fig. 3) because the KBr salt had completely dissolved by the end of the first 4.5-h irrigation period on Day 97 (page 8, lines

14 to 15). In addition, the concentration was assumed to be constant during the application (as no time dependent bromide concentration data were available). Considering bromide infiltration during redistribution of ponding water would, in fact, reduce the application concentration and lead to smaller bromide effluent peak.

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