Hydrology and Earth System Sciences Discussions

Interactive comment on "The dominant role of structure for solute transport in soil: Experimental evidence and modelling of structure and transport in a field experiment" *by* H.-J. Vogel et al.

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We would like to thank Nick Jarvis for his thorough review of our manuscript. He raised a couple of critical points which are worthwhile to discuss in more detail. We would like to split the discussion into more fundamental questions and more technical issues.

Fundamental questions

Relation of our work to other models It was not our intention to doom dual-permeability (DP) models which are in many cases the only practical and physically based way to represent preferential flow along macropores at the larger scale. In our approach, the idealization of structure as required by DP models is replaced by

an explicit but rough representation of the structure which is suposedly relevant for the considered processes. In this way we avoid the estimation of effective parameters which can only be obtained by inverse modeling and which are only meaningful when assuming that the material is macroscopically homogeneous. The price we have to pay is the need of additional information on the structural composition of the material and much more computing power, but we also get a more realistic representation of the flow field. We tried to discuss this point in a more balanced way as suggested by Jarvis.

However we would like to insist on the statement that the parameters required by DP models are in principle dependent on the initial and boundary conditions of the experiment which has to be used for inverse modeling. This can be explained theoretically and it was demonstrated with numerical simulations [*Roth*(1995), *Roth and Hammel*(1996),]. Experimental evidence, however, is scarce because a systematic investigation of solute transport is typically done with high flow rates at high water contents where the hydraulic conductivity is high - simply because time is always short. (The work of [*Kätterer et al.*(2001)] is also restricted to one single flow rate near the saturated conductivity of the material).

We definitely agree with Jarvis that DP-models would predict exactly the same overall behavior as our approach without changing the related DP-parameters, i.e. preferential flow at high flux and matrix flow at low flux. This is true as long as we are dealing with a macroscopically homogeneous matrix and a macroporous structure embedded therein as is the case in the A2 horizon of our field plot. DP-models are conceptual models with exactly this type of structure in mind. But the structure of our field plot is more complex which brings up other aspects. Using our approach we can get much closer to the problem: what does a particle 'see' on its way through soil and this is the relevant aspect for its fate. While this is not an important question if we are only interested in the break-through curve of a non-reactive or linear sorbing tracer, it is of great importance for non-linear

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sorbing solutes and reactive transport. If the structural elements are on a length scale comparable to the scale of interest this structure determines the spatial distribution of solutes and thus, it is highly relevant for reaction rates. It is not clear to us how this can be incorporated in a DP-model.

Applicability of our approach We absolutely concur with Jarvis that the advantages of our approach is not always easy to realize in practice. Actually, as mentioned before, the price might be significant. From Jarvis' comments we conclude however that one important point might have been misunderstood. We definitely do not state that the structure of soil has to be represented explicitly with a precision such that all pores where most flow and transport actually takes place are well represented. In contrast, the message we would like to communicate is that at a given spatial scale only the *rough* representation of the *relevant structure* has to be considered. Where *rough* means 'not in any detail' while important aspects as e.g. connectivity should be considered and *relevant structure* means this part of hydraulically sensitive heterogeneity which has a characteristic length in the size range of the region of interest and which is *not* included in a representative way. The latter would allow to describe the heterogeneity through effective parameters (and we would talk about texture instead of structure). Actually the example brought up by Jarvis is well suited to demonstrate this idea: At the high flow rate in our experiment the macropores become active and they are the dominant structure that is not captured representatively in our experimental plot and which have to be considered explicitly in our model. At the REV-scale of the macropores, they could also be considered implicitly through a DP-model. If the infiltration rate is below the saturated conductivity of the compacted layer, the macropores are not active anymore and the pores most important for flow and transport would be below 1 mm in size and there will be 'more than 10.000' as indicated by Jarvis (actually there will be a continuum of pores, so it is difficult to put a number here) . However the characteristic length of these pores (diameter

and/or characteristic distance between branching points) and herewith the size of a corresponding REV is much smaller than the region of interest, and thus, the contribution of these pores can be represented through effective parameters. For the specific case of our experiment, this means that solute transport at low flux can be predicted based on the hydraulic properties and the geometry of the different horizons (which actually is our scenario $SC_{\mathrm{low-flow}}$) In the same way all the other 'microscopic properties mentioned by Jarvis - aggregate skins, macropore linings - need to be represented by means of effective properties.

To further illustrate the essential difference between our approach and DP-models, we consider the hypothetical case, that there is a coarse textured layer within the flow domain acting as barrier at low flow rates. This might lead to another type of preferential flow where the vertical transport is focused at some locations. While this behavior is generically included in our approach - only considering the rough structure of e.g. soil layers - it is not possible to reproduce this behavior with DP-models calibrated at a high flux. This is also a typical case where DP-model parameters are expected to be sensitive for initial and boundary conditions.

Calibration and prediction Jarvis is right, when he states that we used the information of the dye tracing experiment prior to modeling. But we did not use it in the sense of model calibration. We used it in so far, that we got the qualitative information that there is preferential flow along macropores through the compacted horizon. This information could be obtained also by a much simpler experiment. The actual density of macropores was estimated from field observation also considering the computational ease of simulating a square number of macropores within the square surface. So we decided that in our field plot 9 is more realistic than 16. Actually this approach is in line with our idea that the rough structure might be sufficient.

We would like very much to enter the competition proposed by Jarvis, to carry

out comparative 'blind' model tests to quantify the true predictive accuracy of DP-models and our approach. The test case, however, should be more complex than a simple matrix-macropore structure and a non-reactive tracer, which directly corresponds to the idealization of DP-models, and we should consider different flow rates or, even better, transient conditions which is the rule in nature. Surely, DP-models are doing a good job in situations that correspond to the type of structure they are made for. But we think that our approach is much more general and can be translated also to larger scales. We are convinced that we find 'macroscopic' structure relevant for solute transport at any spatial scale. Macropores are only an example of a highly relevant feature at a very specific scale.

Our intention is to show that very different sources of structure information can be combined to get a better picture of the whole - and finally a better quantitative understanding of flow and transport. This includes a better predictability in situations where the characteristic scale of the relevant structure is comparable to the observation scale. In such situations, which are the rule rather than the exception, effective models cannot be applied in principle. Having this in mind, the statement 'All models are wrong, but some are useful' might be a bit too simplistic. While the first part of this statement is obvious in the sense that all models are an abstraction of reality. For the second part, however, it should be added that some models which are useful in some situations might be dead wrong in another one. Our job is to find the best compromise between a realistic representation of the subject (material and physical processes) and the required input. We agree with Jarvis, that today DP models might be the most complex models, which can be used for management applications, but this is no reason to ignore their limitations.

Technical issues

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Resolution and numerical artefacts We used a relation of 1:1 between the finite-volume size and the radius of numerical macropores. We checked for grid convergence to make sure that a higher resolution would not change the results. The hydraulic parameters we used to model the macropores actually correspond to pores of 0.5 mm as noted by Jarvis, which is somewhat smaller than the actual diameter of the earthworm burrows. In principle it is possible to chose the parameter α such that it corresponds to the actual pore diameter. Doing so, the efficiency of the numerical solver is reduced but the numerical stability is not affected. Because of computational efficiency we keep the lower value for α. We think this is justified as the hydraulic diameter (or resistivity) of macropores in soil is lower (higher) compared to a straight cylindrical tube and, more important, because this choice has no effect on the results. However, it has to be noted, that the critical point for the water potential where macropore flow is induced actually depends on the choice of this parameter. In this case we shifted this critical point from about -0.2 hPa to -5 hPa which is not relevant for our experiment since the water potential at the upper boundary of the compacted layer was ≥ 0. We discuss this point in more detail in the revised manuscript.

Realistic flux Of course, Jarvis is right in mentioning that in this part of France where we did the experiment rainfall intensities of 13 mm/h are rare. However, especially in this region, high corn yields are gained through irrigation which is done at comparable rates. Hence, our experiment provided valuable new insight for the farmer.

Specific comments

1. Of course the detailed flow paths will remain 'unknowable' but if there is some sort of relevant hydraulic structure (not necessarily at the pore level) within the

flow domain and the size of this structure is comparable to the size of the flow domain, there are no meaningful effective descriptions. We tried to reformulate this paragraph to hopefully make this important point clearer.

2. We deleted the word 'ad-hoc'.

3. We deleted this sentence but added the point that the zones of different mobility are considered to have a fixed volume fraction.

4. We added the reference of [*Kätterer et al.*(2001)] and [*Larsbo et al.*(2005)]

5. We toned our statement down as suggested by Jarvis, which does not change the messages that i) parameters of DP-models may change with initial and boundary conditions (actually, [*Kätterer et al.*(2001)] used one single flow rate close to the saturated conductivity) and that they may change with different transport distances as reported by e.g. [*Vanderborght et al.*(2001)].

6. Soil tillage was done using a 'grubber' (this is what the dictionary offers for the translation of the German expression 'Grubber').

7. We changed 'periodically' to 'annually'.

8. We made reference to the work of [*Jarvis et al.*(1987)].

9. We cited the work of [*Gerke and van Genuchten*(1993)] and added a warning about the problem of introducing artifacts further below, where the parameterization is described.

10. We corrected the sign throughout the paper

11. It can be rigorously shown that for $n < 2$ there is an unrealistic steep decrease of hydraulic conductivity when using the approach of [*Mualem*(1976)]. This is because the contribution of unrealistic large pores is overestimated which can be

expressed mathematically through the fact that for $n < 2$ and for $h \rightarrow 0$ the absolute value of the derivative of the water retention curve $\left|\frac{dS}{dh}\right|$ decreases slower than the ratio $\frac{1}{h}$ (the measure of pore size) increases towards infinity. We would like to refer to [*Ippisch et al.*(2006), *Ippisch et al.*(2005)] for more details. There is definitely no trick to adapt the hydraulic properties of the $A2$ horizon to better fit the experimental results. In fact the choice of the air entry value for this horizon is irrelevant for the overall behavior, we just took the measured parameters of the horizon below and we reduced the saturated conductivity (which is more sensitive) and decreased the air entry value to account for the obvious compaction of this material.

12. The linear size of the finite volumes corresponds to the radius of the macropores which was 7.5 mm. This was added to the text.

13. We replaced dispersion by diffusion, but both expressions can be justified.

14. [*Kasteel et al.*(2002),] used a modified Langmuir model to describe the sorption isotherm based on classical batch experiments, we used the simpler Langmuir model with the parameters reported by Kasteel et al. just to get an approximate representation of the non-linear sorption behavior in our soil which was different from that of Kasteel et al.. Moreover we assumed that there is no difference between sorption in macropores and matrix which - we agree - might not be exactly true and we added a note to the revised manuscript. However, we demonstrated the effect of sorption through different scenarios with and without sorption. We think that in this context, a deeper discussion how the parameters are measured by Kasteel et al. is not required. The Langmuir isotherm was then used with the classical convection-dispersion model:

$$\frac{\partial C_{tot}}{\partial t} + \nabla \cdot (C_w j_w - D_0 \nabla C_w) = 0$$

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and

$$C_{tot} = \theta C_w + C_s = \theta C_w + \frac{C_s^\infty \, k \, C_w}{1. + \theta k C_w}$$

15. Yes, this was a misleading sentence. Surely the lack of macropore flow is the critical point, there is only an additional effect due to the non-linear sorption.

16. We reworked that paragraph as already discussed in the general discussion above.

17. We added a sentence that our statement is true for materials which are not macroscopically homogeneous, i.e. materials that do have macroscopic structure as defined in the introduction.

18. The saturated conductivity of macropores was calculated with Poiseuille's law for a pore diameter of 0.5 mm. This parameter, however, is not sensitive for the simulations. We added a note in the revised manuscript also explaining that either α or h_e is relevant for the air entry pressure which is now also indicated in Table 1. The whole parameter set was the result of inverse modeling based on the multi-step outflow experiments which actually are quite sensitive to the hydraulic conductivity close to saturation. Also the conductivity of 180mm h^{-1} at a water potential of -10.2 cm is obtained in that way. Two figures showing the data of the multi-step outflow experiments together with the results of inverse modeling using standard van Genuchten parametrization and the modified version we used are available at www.ufz.de/index.php?de=7019 . Actually the data are well described by the model. There could be a slight overestimation of hydraulic conductivity in the pressure range between -10 cm and -20 cm because the shape of the outflow steps is more gradual in the experimental data compared to the model.

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