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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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This paper deals with numerical modelling of water flow and solute transport in structured soil, where the structural pores (in this case earthworm channels) are explicitly described. The simulations are based on information on flow pathways obtained from a dye tracing experiment, and field data on hydraulic properties measured nearby. The results of the study can be summarized by the classic phrase: 'the model simulations are in reasonable agreement with the measurements!'. First of all, I would like to strongly commend the authors on the emphasis they place on the importance of linking soil structure to solute transport modelling. I couldn't agree more that this connection is critical. I also greatly appreciated the 'genetic' technique based on percolation theory, which they used to generate the description of soil macropores, and the way this was

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combined with Miller scaling to account for heterogeneity in the matrix. This is certainly pragmatic and novel, and the conclusion that textural heterogeneity is not important in the presence of macropore flow is important. All in all, the paper will make a useful contribution to this research field. However, it is the job of a referee to be critical, and so I feel I should mention some areas of the paper that could be strengthened. I don't have any significant concerns about the actual work carried out, but I do feel that the paper lacks a little balance and perspective when the authors attempt to relate their own work to that of others. I will try to explain what I mean in the following. My comments consist of a general discussion and review of some of the very important and interesting wider issues that have been raised by the authors in their paper, followed by some specific points of clarification.

General comments: The authors adopt what might be called a hybrid 'discrete pore-continuum' approach, where individual macropores (earthworm channels) are treated as discrete geometric objects in the model, but they are represented numerically as a pore continuum. I personally find this mix of concepts a little confusing. For example, it would be very interesting to know the size of the finite-volumes used in the numerical modelling, in relation to the size of the numerical macropores (7.5 mm diameter, line 21, page 2164). It may be already somewhere in the paper and I missed it, in which case I apologize! I can also imagine that this approach might easily generate numerical artefacts if inappropriate hydraulic functions are chosen to represent what are really discrete pore features. However, I am willing to accept that it can work reasonably well in practice, providing special care is taken in specifying the macropore hydraulic properties in the Mualem-van Genuchten model. I am not sure the authors have succeeded perfectly with this. It seems from their choice of parameter values for the macropore region (table 1) that hydraulically-speaking they are modelling macropores roughly 0.5 mm diameter even though the worm channels in reality were 7.5 mm in diameter. I suspect this may be due to numerical stability problems that would arise if van Genuchten's a was set to a more appropriate value for 7.5 mm diameter pores ($>$ 1 cm-1) at the same time as the n value is (quite correctly) set to a very large

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number (8). I think the authors should discuss this issue, because it may have some implications for the practical applicability of the method.

The authors compare and contrast the perceived advantages of their approach to existing models, which they criticize strongly. Actually, in several places in the paper (e.g. p.2170, lines 13-16), it is not completely clear to me what kind of existing models are being criticized, but in the following I will assume that dual-permeability (DP) models are the author's main target! They suggest that because DP models use an 'effective' description of soil structure, they must always be calibrated, can never be used predictively, and will fail when the initial and boundary conditions change. However, I feel that the authors tend here to exaggerate the problems with other approaches, while glossing over some equally important limitations in their own. A more balanced perspective in the discussion of the various advantages and disadvantages of different modelling approaches would greatly improve the paper. I will try to illustrate what I mean in the following paragraphs.

Although individual structural pores are not explicitly simulated, DP models do account for an 'idealized' soil structural geometry in a one-dimensional framework. The mass exchange coefficient, which expresses the strength of lateral mixing in the soil, can be directly related to aspects of this idealized geometry (i.e. half the aggregate width, or the spacing between macropores, for example, see Gerke & van Genuchten, 1996). One potential problem with DP models is that the first-order assumption underlying the description of mass exchange is only an approximation, and it is true that the value of the coefficient may depend in an unknown way on initial and boundary conditions (e.g. Griffioen, 1998). However, it seems that this kind of 'model error' may not always be so critical in practice, especially considering the many other uncertainties involved in simulating solute transport in naturally structured soils. For example, Kätterer et al. (2001) showed that a single parameter set in a DP model could successfully simulate tracer experiments carried out under widely different initial and boundary conditions. The only failure in their study was related to the occurrence of water repellency, which

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was not surprising since this process was not included in the model.

In a three-dimensional discrete-pore model, a more complex, flexible and variable geometry can be defined separately for each individual macropore, and there is, on the face of it, no need to make any approximations or assumptions about mass exchange between macropores and matrix. However, I am not convinced that these advantages are easy to realize in practice, at least not with the computer power and observational techniques available today. Real soil structure is much more complex than any model can describe explicitly: the authors have simulated at the small plot scale, the effects on flow and transport of a few 7.5 mm diameter earthworm channels (density 9 m-2) activated by steady irrigation at an intensity of 13 mm h-1. The authors point out many times in their paper that changing boundary conditions will change the flow and transport pattern, which is certainly true. In many climates (certainly in France anyway), 13 mm h-1 is a high rate for natural precipitation (especially sustained for such a long time). Dye tracing experiments under controlled tensions (Jarvis et al., 1987), as well as measurements of near-saturated hydraulic conductivity (e.g. Jarvis & Messing, 1995) suggest that at more typical lower rainfall rates, earthworm channels 7.5 mm in diameter would remain air-filled (good news for the worms!) and preferential flow and transport takes place in smaller macropores and mesopores that are more densely distributed (see Luxmoore et al. 1990). If we take as an example pores with equivalent diameters of between ca. 0.3 to 0.6 mm (roughly the same size pores, hydraulically, as simulated in this paper), and make the reasonable assumption that they constitute 1% of the porosity, there will be more than 10,000 such pores in each m2 of soil, although not all will be hydraulically active. This is a sobering thought, as I can imagine that it would be a major challenge, both numerically and experimentally, to account for the attendant geometric complexity of such a pore system in a discrete-pore model. The authors do give an example in the paper of the effects of boundary conditions on transport behaviour, demonstrating that their model responds to a reduction in the irrigation intensity from 13 to 1.3 mm h-1 by eliminating macropore flow and transport, reducing the flow regime to homogeneous matrix flow. This is fine, and exactly as it should be, but the authors seem to imply that DP models could not do the same thing without changing (re-calibrating) parameters (page 2170, lines 18-19). This is not correct: any physics-based DP model would predict exactly the same behaviour without needing to change any of the parameter values. If the applied flux (in this example 1.3 mm h-1) is less than the saturated matrix conductivity (2.9 mm h-1 in the A2 horizon, table 1), then clearly only matrix flow will be simulated. Thus, as long as discrete-pore models employ 'rough' descriptions (in the authors own words) of real macropore systems in soils, they will just predict the same behaviour as dual-continuum models. They may even be less effective than DP models for real-world applications under natural boundary conditions, if only a few large macropores can be included in the model for practical reasons. In this case, preferential flow will only be occasionally triggered in the model (much less often than occurs in reality), since the required high intensity storms are few and far between. It might be possible to get around this problem by manipulating the hydraulic properties, but then the whole point of explicitly describing individual pores is lost.

Even if it did become practical sometime in the future to completely and explicitly describe the complex geometry of thousands of soil macropores and mesopores at the m2 plot scale, there are additional aspects of soil structure that I suspect would probably make the effort futile: micrometer to millimetre thick aggregate skins ('cutans') and macropore linings are known to have very different hydraulic (Gerke and Köhne, 2002), biological (Pivetz & Steenhuis, 1995; Mallawatantri et al., 1996) and chemical (Turner and Steele, 1988) properties compared to the bulk soil matrix, which in turn strongly influences interaction between flow regions and overall transport behaviour (Anderson & Bouma, 1977; Thoma et al., 1992; Stehouwer et al., 1994; Pivetz et al., 1996; see also my specific comment no.14). It would be a major challenge to satisfactorily incorporate these aspects into a complete geometry-explicit description of soil structure effects on transport. Ignoring these effects, as the authors have done in their paper, must surely overestimate the strength of interaction between water and solutes in a single macropore and the surrounding matrix. I suppose that this could be compensated by other approximations, for example an underestimation of the number of conducting preferential flow pathways (Fig. 4 seems to provide some visual evidence for just such a compensation). However, I can't then avoid the general feeling that the 'rough description' of soil macropores included in the model (due to practical constraints) inevitably leads to an 'effective' description of the influence of structure on solute transport, one that is in practice no different to DP models.

My final comments concern the nature of calibration and prediction. It's perhaps true that, in a very strict sense, the authors did not calibrate their model. But in order to construct their conceptual model, they did make use of the visual impressions gained from a dye tracing experiment carried out on the soil block they modelled. It could be argued that in practice, this is effectively the same as calibration, since it seems that to construct and apply the model we need to conduct a dye tracing experiment, and then dig up the soil to see what happened (see page 2162, lines 21-22). It would be interesting to see how well their model could truly predict transport based on descriptions or measurements of soil structure without the benefit of first staining the flow paths with dye. The nature of the individual flow paths will then be unknown (and in principle 'unknowable'), since only a small proportion of macropores are hydraulically active. In this situation, I can't see any reason to expect that predictions of state-of-the-art discrete pore models would be generally better than their counterpart DP models. In fact, I think it would be very interesting to carry out comparative 'blind' model tests in order to quantify the true predictive accuracy of different approaches!

Of course, computer power is continuously increasing and experimental techniques to observe and quantify soil structure are also improving. In the (distant?) future, this might lead to significant advantages for discrete-pore models compared to DP models (although I remain sceptical). In the meantime, managers and policy-makers cannot wait, since they need useable modelling tools today that can account for preferential flow and transport. DP models are now being used for many different predictive management applications (e.g. pesticide regulation in the EU, see also Vanclooster et al.,

2004) due to their relative operational simplicity and because their performance is perceived to be good enough for the purpose at hand. As the saying goes, 'All models are wrong, but some are useful'!

Specific comments

1. p. 2155, lines 1-12. I'm not sure I understand what you are trying to say here. I think we understand the processes well enough (from a physical point of view), but it is difficult to make accurate predictions because the geometry of the flow paths is unknown, and will remain 'unknowable' for purely predictive applications, since we can't dig up every piece of soil we want to simulate.

2. p.2155, line 26. Please delete the word 'ad-hoc' here. It is the wrong word in this context. All models are simplifications.

3. p. 2155, lines 27-28. Delete the text 'with the idea..of the porous network'. That might be true of the first reference cited here, but not the other two.

4. p.2156, line 2. After 'quite accurately'. Can you add a reference or two here?

5. p.2156, lines 7-12. You might expect the parameters to change, but in practice this may not happen. For example, Kätterer et al. (2001) showed that the same parameter set could be used to simulate transport experiments with widely different initial and boundary conditions (the only failure in their study was related to the occurrence of water repellency, since this process was not included in the model). You should tone this down by replacing 'are expected to change' by 'may change' on line 8: Further, I cannot see anything in Vanderborght et al. (2001) that would per se invalidate the use of dual-permeability models. The effects of vertical soil heterogeneity related to differences in structure and texture can be accounted for by different lateral mixing rates (= mass transfer coefficients) in the different horizons. The increasing effective dispersivity with flow rate is also roughly reproduced in DP models in a two-region sense, rather than the more advanced multi-region approach demonstrated by Vanderborght et al. In DP

models, the effective dispersivity will be constant as long as the applied flux remains below the saturated matrix conductivity, but will increase when flow is triggered in the macropores at larger fluxes. Summarizing, on line 11, I think you should change 'cannot be used' to something much less categorical, like 'predictions for conditions other than those the models are calibrated for, may be uncertain'. We can always make predictions, the question is how accurate will they be?

6. p.2158, line 15. What is a 'gruber'? Maybe you mean a shallow 'tine' or a disc harrow?

7. p.2158, line 16. Should this be 'annually', rather than 'periodically'?

8. p.2164, lines 22-25. Yes, this aspect is very interesting. If you want to see how this might influence transport, you could also check out the results of the dye tracing experiment reported by Jarvis et al. (1987).

9. p.2165, line 16. You could also cite others who have done the same (e.g. Gerke & van Genuchten, 1993), and perhaps also warn of the dangers. The macropore unsaturated conductivity is very sensitive to the van Genuchten parameters assumed here, and it is easy to introduce artifacts.

10. p.2165, line 19. You mix up tensions and pressures here (and throughout the paper). Since h is positive, you should write tension.

11. p.2166, lines 4-9. I think you should briefly explain for the reader why it is unreasonable, since this is not widely appreciated (simply because there should, in principle, be a maximum pore size in soil). But actually, this does not seem to me to be the most important reason for introducing this 'cut-off' in your work, evidenced by the fact that (apart from the macropores) you set the air-entry pressure quite a long way from saturation (table 1). In fact, you also use this concept to define the matrix-macropore boundary (see also Larsbo et al., 2005), to ensure that the matrix does not get assigned hydraulic properties more appropriate to macropores. I think you should also

clarify this for the readers.

12. p.2166, line 22. What size are these finite volumes?

13. p.2167, lines 7 and 9. Perhaps you should replace the word dispersion with diffusion?

14. p.2167, line 12. It is not clear to me i.) how the parameters of the sorption isotherm were determined, and ii.) how sorption was incorporated into the advection-diffusion model. You shouldn't expect readers to go to Kasteel et al. to find the answers, since these are not trivial issues. For example, we should not expect sorption to be identical in macropore and matrix regions, due to widely different surface areas available for liquid-solid interactions. Perhaps you tackled this by assuming a much lower bulk density in the macropore region? Anyway, some discussion of this point would be a good idea, because the extent of sorption retardation in the macropores is a critical control on transport.

15. p.2170, line 9. I don't understand this sentence. Surely, the lack of macropore flow in the SClow-flow scenario is the critical point?

16. p.2170, lines 10-19. As mentioned in the general discussion above, this text is misleading and should be re-worked. DP models would predict the same contrasting behaviour between SClow-flow and SCreference, without any change of parameter values.

17. p.2171, lines 16-21. I hope that you can re-phrase this conclusion, in the light of the general discussion above. However, I do strongly agree with the sentiment that we must consider soil structure in solute transport modeling.

18. How was the saturated conductivity of 3600 cm/hour estimated (table 1)? You must have had some basis for this estimate, which I think you could share with the readers. I know the macropores in your model are not straight-sided cylindrical tubes, but how does this number compare to what would be calculated for 0.5 mm (and 7.5 mm) diam-

eter pores from Poiseuille's law? This comparison might help. Related to this, it is also a little strange that the soil matrix in the A1 horizon was given a much larger a value (33 cm-1, table 1) than the macropores. I know this has not affected your results, because the conductivity function was 'cut-off' at the air-entry tension (10.2 cm), but it could be confusing for the reader. Even though I haven't seen the original data that you fitted to, I would not be at all surprised if this is a result of fitting the Mualem-van Genuchten functions to data that are strongly influenced by the presence of macropores. This is not a good idea if the functions are subsequently used to characterize the matrix. Jarvis et al. (1999) give a good demonstration of the dangers. One final comment concerning hydraulic properties in the A1 horizon: although you don't show us the raw data, the conductivity at 10.2 cm tension (180 mm h-1, table 1) does seem extremely large, at least compared to measurements for other similar soils in the literature. I find it hard to believe any soil could be so permeable when pores larger than ca. 0.3 mm are excluded from flow. This is also relevant for the B horizon.

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