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Discussions

Interactive comment on "An effective parameterization to quantify multiple solute flux breakthrough curves" *by* E. Bloem et al.

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Response to first point made by referee 1: Multi-compartment samplers allow the breakthrough curve of a large soil volume to be separated into the breakthrough curves of the soil volumes enveloped by the stream tubes that exit in each of the sampling compartments. Solute passing through these tubes experience longitudinal dispersion as well as transversal dispersion. Because the sampling cells are small and the soil volumes exiting into them are not isolated, the transversal dispersion quickly leads to solute changing from one stream tube to another, thereby ending up in another cell.

When this transversal dispersion is effective, dissolved substances experience a wide range of flow velocities, and the solute transport in the soil volume as a whole will

be convective-dispersive. In the absence of transversal dispersion, solute particles are confined to the stream tube into which they entered when they infiltrated, which is consistent with stochastic-convective solute transport (see Jury and Roth, 1990, Chapters 2 and 3, and Flühler et al. (1996) for an in-depth discussion).

In multi-compartment experiments the observed breakthrough curve of a particular sampling cell reflects various sources of solute dispersion:

1)Longitudinal dispersion of solute particles that never left the stream tube. These are the particles that during infiltration entered the stream tube connected to the sampling compartment through which they excited the soil.

2)Particles entering the stream tube from neighboring stream tubes. These particles initially traveled through a (faster or slower) stream tube and entered the stream tube at some point between the soil surface and the sampler, and did not leave the stream tube before entering the sampler. This is a form of transversal dispersion that adds solutes to the stream tube. The probability of solute particle entering the steam tube is higher at location where horizontal concentration gradients are positive in horizontal directions moving away from the stream tube (lower concentrations inside the stream tube than in its immediate surroundings).

3)Particles leaving the stream tube towards neighboring stream tubes. This mechanism is similar to 2), but in the opposite direction. Negative horizontal concentration gradients are conducive to this mechanism.

4)Particles that wandered around so profusely they entered and left the stream tube repeatedly, and the exiting stream tube is more or less random. This is the case when the sample is much deeper (> 10 times) than the soil's dispersivity measured at the scale of the sampled volume above the multicompartment sampler, not that of an individual stream tube.

Note that 2) and 3) generally work to reduce lateral concentration gradients and flatten the breakthrough curve of an individual stream tube compared to that of a fully isolated stream tube. Once the lateral gradient is completely eliminated (a condition approximated best when condition 4) has been achieved), the solute transport process in the soil volume can be considered purely convective-dispersive. In that case, the breakthrough curves of all compartments expressed in flux concentrations would be identical. When expressed by amounts of solutes leached, the vertical scale of any of the data point on those curves would be determined by the volume of water of the sample of that sampling compartment during that sampling interval and the uniform flux concentration during the sampling interval. Thus, the breakthrough curve of an individual cell does not say very much about the nature of the solute leaching process of the soil volume as a whole, and not even about the processes within the individual stream tube since we cannot separate mechanisms 1 through 4 listed above. That being said, in order to parameterize the leaching surface we had to find a curve that provided and adequate fit and we found that the solution to a 1D steady-state version of the CDE provided this. The fitted BTCs are produced by a combination of the first three mechanisms above (the fourth already is a combination of 2 and 3), while the CDE was designed to adequately describe only condition 1 and 4. We neither claim nor imply that the fitted parameters can or should be used to describe the transport process in the soil volume as a whole.

If one is interested in interpreting solute leaching data to infer the solute transport process one needs at least two sampling depths for single-cell solute sampling. The spacing between the two can be prohibitively large if the shape of the deeper breakthrough curve is compared to curves predicted by convective-dispersive and stochastic-convective models (e.g., Jury and Sposito, 1985). The convective-dispersive model predicts the standard deviation of the solute spreading to increase with the square root of depth whereas the stochastic-convective model predicts a linear increase. Consequently, when the increase of spreading with depth is analyzed, the two depths can be much closer to one another (Vanderborght et al., 2001).

With multi-compartment samplers, the flow regime can be identified with data from a single depth, through dilution theory. De Rooij et al. (2006) present the adaptation of dilution theory for multi-compartment samplers that underlies this approach and illustrate it on data from a multi-compartment lysimeter. This method does not require the assumption of piston flow within individual stream tubes that gives rise to the qualifier 'convective' in the stochastic-convective model. It determines the theoretical values of the dilution index for convective-dispersive and stochastic-convective transport, and places the dilution index calculated form the observation on the continuum scale between these two extremes. It should be noted that there is no direct relation between the quality of the fits to individual breakthrough curves by a CDE-based model, and the nature of the transport mechanism revealed by an analysis of the full leaching surface. Our use of the CDE for individual breakthrough curves should therefore not be viewed as implying a convective-dispersive transport mode, but simply as a flexible parameterization of the individual breakthrough curves, whatever the mechanisms that produced them.

Flühler, H., Durner, W., and Flury, M.: Lateral solute mixing processes – a key for understanding field-scale transport of water and solutes, Geoderma, 70, 165-183, 1996. Jury, W.A., and Roth, K.: Transfer functions and solute movement through soil. Theory and applications, Birkhäuser Verlag, Basel, 226 pp, 1990. Jury, W.A., and Sposito, G.: Field calibration and validation of solute transport models for the unsaturated zone. Soil Sci. Soc. Am. J., 49, 1331-1341, 1985. Vanderborght, J., Vanclooster, M., Timmerman, A., Seuntjes, P., Mallants, D., Kim, D.-J., Jacques, D., Hubrechts, L., Gonzales, C., Feyen, J., Diels, J., and Deckers, J.: Overview of inert tracer experiments in key Belgian soil types: Relation between transport and soil morphological and hydraulic properties, Water Resour. Res., 37, 2873-2888.

Response to second point made by referee 1: We agree with the reviewer with respect to include information about the uncertainty and will add those in the revised version.

Response to third point made by referee 1: Also a schematic figure to increase readability as proposed by referee 1 can be added to the revised version.

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 11, 6993, 2014.