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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 referee 2: The main difference between the method discussed in Bloem et al. 2012 and this method is the direct parameterization of the leaching surfaces. We apply the parameterization directly to the flux densities (instead of flux concentrations) resulting in one single equation describing the entire leaching surface, while in Bloem et al. 2012 an extra step was needed to arrive at the final leaching surface.

Referee 2 argues that the CDE fits most breakthrough curves. This is one of the reasons it serves our purpose so well: we seek a parameterization that adequately fits all individual BTCs of the compartments in order to make the parameters of these curves functions of the spatial coordinate of the leaching surface. As we explained in

our reply to referee 1, the fact that individual curves can be described well by a solution to the CDE does not imply the transport processes at the scale of the sampler obeys the CDE.

Dr. Koestel chose to classify our leaching surface parameters as 'fudge factors', and noted that they were strictly empirical. One has to keep in mind a few aspects though:

1) the shape of the leaching surface is decidedly non-trivial. Given the fact that a straight-forward plane surface requires three parameters, pinning down something as complicated as the leaching surface with 4 to 8 parameters is an achievement that should not be underestimated. These 'fudge factors' summarize hundreds, sometimes thousands of data points in very many breakthrough curves (100 in this case). Before writing off our parameters as 'fudge factors' one should keep in mind that 200 parameters would be needed if one were to describe each individual breakthrough curve of our multi-compartment samplers, without its relation to any of the other breakthrough curves. We very much doubt a more efficient scheme can be found.

2) The theory behind the mean velocity and the dispersivity as parameters to describe individual breakthrough curves is well established, including its fundamental strengths and weaknesses. Therefore we do not think that Dr. Koestel refers to those as being strictly empirical. The parameters we use to link these breakthrough-curve parameters to the transformed spatial coordinate are indeed empirical. We do not see why this is a fundamental objection against our parameterization. These parameters fulfill the same role as the parameters used in various regression techniques for curve-fitting. We added a dimension and fitted a curved surface instead of a curve. If one readily accepts empirical (or simply convenient) parameters during curve fitting, why should this then be problematic when fitting a curved surface? As more leaching surfaces (from observations or 3D models) become available, it will be possible to study the relationship between the leaching surface parameters and the properties of the flow and the porous medium, but before we can embark on such an endeavor, we need to have a parameterization first.

3) The use of the Beta distribution to describe the distribution of the total leached solute as a function of the transformed spatial coordinate is sensible: many pdfs have infinite or semi-infinite support and thus cannot be used for this purpose. There really is no viable alternative.

We are discussing various potential ways to address the final comment of referee 2 to use the three multi-compartment sampler datasets for additional characterization. Among the possible inclusion of additional novel analyses we are considering the exploration of the relationship between the leaching surface parameters on one hand and the reactor ratio and dilution index on the other. A more remote possibility is to use the parameterized leaching surface to carry out an analysis of the residuals between the data and the fit.

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