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Interactive Comment

Interactive comment on “The backward Îto method for the Lagrangian simulation of transport processes with large space variations of the diffusivity” *by* D. Spivakovskaya et al.

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General: The paper reviews the random walk method as it applies to the simulation of advective dispersive transport in surface water. Standard random walk methods have their basis in stochastic calculus. This calculus applies when coefficients (velocity and dispersion tensor) are smooth functions of space. The focus of the paper is on the use of the "backward Ito" method to treat cases where the dispersion coefficient (or tensor) is characterized by step functions (discontinuities) in space. Although in surface water the dispersion field is generally considered to be continuous, it may be characterized by large gradients that practically appear as discontinuities in the field when the system is discretized for numerical simulation. Even without such large gradients, numerical simulation of flow can result in discontinuities in the velocity field (depending on how the nodal velocity solution is treated), and therefore the velocity-dependent dispersion tensor, as explained below.

Interpolation as an Alternative: The presence, or lack, of discontinuities in the latter case depends upon how velocities from the flow solution are treated in the random walk method. Velocities can be interpolated to generate a smooth dispersion field. In this approach, interpolation methods for the advective components and the dispersive components do not necessarily have to be the same. This is important where cell-by-cell mass balance for flow is associated with a particular interpretation of the numerical solution for the velocity field that may not yield a smooth dispersion field. In this case, a different velocity interpolation method might be used when computing the dispersion tensor. It would be helpful if the authors were to mention these alternative approaches to solving these problems where the dispersion tensor appears discontinuous (see LaBolle, E.M., G.E. Fogg, and A.F.B. Tompson, Random-Walk Simulation of Transport in Heterogeneous Porous Media: Local Mass-Conservation Problem and Implementation Methods, Water Resour. Res., 32(3), 583-593, 1996).

Can't One Simply Refine the Time Step? The assumption by referee 1 that all methods should converge to the same solution if dt is chosen small enough is guaranteed only for a smooth dispersion field. To achieve this when the flow field is solved numerically, the field must be defined as smooth from the nodal velocity solution and the spatial discretization of the numerical solution must be refined along with dt to improve convergence.

Terminology: The application of stochastic calculus assumes a priori that the parameter fields are smooth. For discontinuous coefficients, the usual stochastic calculus does not apply. Thus, rather than use the term "backward Ito" (BI), I would instead use the term “generalized SDE”, “generalized BI”, or something similar.

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Not Simply a Problem of Terminology: This problem is important because equivalence for smooth coefficients between two SDEs (one with and one without gradients) does not necessarily guarantee convergence of the SDE without gradients when then applied to the case of discontinuous coefficients. LaBolle et al. (2000) proved convergence of the "generalized SDE" in one dimension and demonstrated convergence in two dimensions. The usual stochastic calculus could not be used for that proof. For this reason, the applicability of the generalized SDE and its associated random walk method to the problem of discontinuous coefficients has not been demonstrated elsewhere (e.g., within the seminal works of Ito and Stratonovich). Note that the multidimensional form of the generalized SDE developed by LaBolle et al. (2000) is considerably more complicated than the one-D form. Furthermore, in one- and two-D, these problems are constrained by unique eigenvectors. It may be, however, that convergence of the generalized SDE is sensitive to the choice of eigenvectors, which can be non-unique in 3-D.

Example: To emphasize the importance of these apparent subtleties, note that some forms of the methods originally posed by LaBolle et al. (2000) also included a porosity term (for use in transport in porous media). However, the one-D proof by LaBolle et al. (2000) did not include this porosity term. The porosity term was added under the assumption that if gradients could be eliminated in the formulation with porosity, the method would converge for discontinuous porosity; in other words, it was assumed that if the BI converges when coefficients are smooth, then the "generalized BI" converges when they are discontinuous. Examples with small porosity contrasts typical of alluvium suggested that this assumption was correct. Since then, it has been noted that for large contrasts in the porosity, the method breaks down (LaBolle, E.M. and Y. Zhang, Reply to Comment by Doo-Hyun Lim on "Diffusion processes in composite porous media and their numerical integration by random walks: Generalized stochastic differential equations with discontinuous coefficients", Water Resour. Res.,42(2), 2006). The porosity problem is not an issue for the current application, and LaBolle and Zhang (2006) showed that good results can be obtained by treating porosity as

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a smooth function of space. Nevertheless, this problem illustrates the need to treat these equations in a class by themselves - they are not technically stochastic differential equations when discontinuous coefficients are used. The stochastic calculus does not apply and convergence must be tested or proved for a given formulation. In my opinion, minor modifications to the terminology and discussion should convey these subtle, but important aspects of the problem.

Interactive comment on Ocean Sci. Discuss., 4, 623, 2007.