RC2: 'Comment on hess-2023-131', Anonymous Referee #2, 18 Sep 2023

The manuscript develops an adjoint subordinated fractional-dispersion equation (S-FDE) in order to estimate release times and source locations of contaminants in aquifers and rivers. The author first (Section 2) present the three-dimensional forward S-FDE and then derive its adjoint following the approach of Neupauer and Wilson and using fractional-order integration by parts, and a fractional-order extension of the divergence theorem. Then, a Lagrangian backward solver is presented based on the developments of the lead authors. The solver is validated by comparison to finite difference solutions of the S-FDE. In Section 3, the developed backward tracking methodology is then applied to three field scenarios to estimate the release history of pollutants, and groundwater age. Section 4 discusses extensions of the proposed method to identify pollutant source locations, and multi-scale subordinated models, relevant for fractured media. This is an interesting contribution that adds to the literature on S-FDEs and source and release time identification in aquifers and rivers. In the following, I list a few comments and recommendations:

Comments:

(1) Line 103: Could the authors give a physical explanation of the meaning of the space-fractional advection term and the subordination to the velocity field? This is important because in field applications, solute transport is typically advection-dominated.

Reply: We thank the reviewer for offering helpful feedback that improved the presentation of this work. In the revised manuscript (lines 120-124), we added the following explanation regarding the subordination term in Eq. (1a), which can be directly equated to the space fractional derivative when the equation simplifies to one dimension:

"*It is worth noting that pollutant particles undergo advective displacement controlled by local mean velocity, with individual particles migrating along various flow paths in a heterogeneous medium, leading to random mechanical dispersion due to local speeds deviating from the mean velocity. Eq. (1a) assumes a (tempered) α-stable density distribution for random mechanical dispersive jumps, rescaled by the mean local velocity. This (tempered) α-stable density encompasses both Gaussian and power-law densities as two end members.*"

(2) Line 126 and following: The detailed derivations could be moved to an appendix.

Reply: Done. We moved the detailed deviations to Appendix A.

(3) Lines 123-124: It is not clear what the authors mean here. Molecular diffusion should model hydrodynamic dispersion? I assume the space fractional derivative should account for dispersion. This should be clarified.

Reply: We revised this statement (lines 267~268), and it now reads as follows:

"*Notably, if molecular diffusion is not negligible, it can be included in Eq. (1), combining with the subordination term responsible for mechanical dispersion to define hydrodynamic dispersion.*"

We concur with the reviewer that the space fractional derivative explains super-diffusion resulting from rapid displacement along preferential flow paths, which can typically overshadow molecular diffusion's influence on particle dispersion.

(4) Lines 146 and 152: When the authors refer to fractional-order integration and integration by parts of the spatial derivatives, do they mean the use of the divergence theorem and its fractional-order extensions? This should be clarified.

Reply: We used integration by parts, whether fractional or integer order, rather than the divergence theorem. For instance, Eq. (5) (now Eq. (A2)) employed fractional-order integration by parts, which doesn't involve vector field flux through a closed surface. Eq. (6) (now Eq. (A3)) applied integer-order integration by parts in the first equality and the Green's divergence theorem in the second. We clarified this in the revised manuscript (line 717).

(5) Section 2.2: This section refers extensively to previous work by the lead author. It would be instructive for the reader if the authors could provide the Lagrangian equations that are implemented in the solver.

Reply: Done. We added the temporal Langevin equation that describes the non-Markovin displacement of solute particles over time in the revised manuscript (lines 259~262).

(6) Lines 297 and 302: What is meant by relatively homogeneous/heterogeneous? How are the K-fields generated and how are they characterized (log-K variance, correlation length, etc.)?

Reply: We generated the K-fields using the 2D fractional Brownian motion (fBm) random field method developed by Zhang et al. (2019a). Particularly, log-normal random K values were distributed in space using the Fourier filter function. The Hurst parameter in the filter function defines the spatial correlation of K values: a relatively 'homogeneous' K-field exhibits weak correlation (e.g., Fig. 2a), while a 'heterogeneous' K-field displays strong correlation (e.g., Fig. 2c). We have included this clarification in the revised manuscript (lines 324~326).

(7) Line 300: Do the authors add diffusion to capture hydrodynamic dispersion? This needs to be clarified.

Reply: Yes, we have done this. It's necessary because molecular diffusion is a component of hydrodynamic dispersion. Please see also our response for Question 3.