Reviewer comments (RC2) in black and answers in blue

General Comments

A new method proposed here would allow a faster ranking of geological multiple scenarios in ground water contamination problems by replacing the grid model per graph and the transport solver within partial differential equations by metrics on graph.

- The details given in the article would allow to reproduce the method by others.
- The article is clearly structured, containing the state of art (introduction), method description and results discussion. The application to a synthetic case is appearing from the beginning of the “Method” part, but since the illustrations on this single application case are helping to understand and to follow the method, it stands well where it is.
- Overall, I appreciate the open discussion where the authors are evocating the remaining challenge of the choice of the threshold or the choice of the particular metrics.

Thanks for your positive comments.

General Suggestions

- As far as I understood, the grid is replaced by a graph with no loosing information, where each cell center is replaced by a node and the conductivity between neighbor cells as replaced by a directional edge. Can you state more clearly on that fact in your work, precising that the support of information being change (grid to graph) but with identical information and resolution ? Do you use all cells of initial model to create a graph or you neglect the flank cells never participating in the flow? Clarify please that there is no upscaling nor graph reduction here and so it is a perfectly bijective transformation. One it is said, would it mean the heart of your approach is not in grid to graph transformation but in the proxy of flow simulator ?

  Yes, this is correct. We can precise that we use all cells of the initial model, keep identical information and resolution, and that there is no upscaling nor graph reduction. We will add these precisions at the revision of the manuscript in section 2.2.

- For the same clarity purpose, I would separate the replacement of grid by graph step from the step of replacement of the flow-transport simulator by a proxi with graphs metrics computation. In more general application, the Dijkstra or other graph metrics algorithms may easily by applied to a grid support and get the same results (since the transformation from grid to graph is bijective and finally just a question of format of the data).

  Each of these two steps already have its own subsection 2.2.1 Graph generation (for the replacement of grid by graph step) and 2.2.2 Computation (for the step of replacement of the flow-transport simulator by a proxy).

- In case if the transformation to the graph is crucial for this work, please argue this and demonstrate that the following algorithms would not work elsewhere.

  Dijkstra's algorithm finds shortest paths between nodes in a weighted graphs. This is why it is crucial to format the geological model as a graph. We will add this clarification before section 2.2.1 at the revision of the manuscript.

- I would place the information in Appendix A in the beginning of the methodology description. As I understood, the proposed approach is performing less good in more homogeneous media. It is not a blocking point itself, but you need to demonstrate that for the other same conditions and the same "matrix" media, your approach do perform differently in the case where you have contract heterogeneities (with and without faults).

  We prefer to keep this part in appendix as it does not contribute to address conceptual uncertainty exploration and scenario selection which is the main motivation of this work. As explained in Appendix A, the absence of very high conductivity paths (or very low conductivity barriers), which the graph approximates quite well can explain the mitigated performance of a graph-based approach in a multi-Gaussian setting. So, the use of the method is particularly interesting to tests scenarios displaying different types of hydraulic conductivity contrasts or pathways. This explanation will be added to the discussion at the revision of the manuscript.

- The calibration of the threshold on the distance map for your methodology should be done using the parallel with the conventional flow-transport results (with MODFLOW). It is understandable that for the brand-new approach such calibration could be needed. But for the eventual industrial use of your approach, would your approach will depend on the conventional result or you may envisage another calibration process?

  We do not envisage other calibration methods at the moment. Nonetheless, the calibration can be conducted on a limited number of scenarios for a specific setting. It would still allow for the exploration of additional scenarios. We would be keen to hear about alternatives.

- The fact that you are using an oriented graph does limit you to apply your approach to the highly connected media ? This is the reason why your fractures are not connected to each other in your synthetic example ? If such is the case, please discuss it in the limits of your approach application. What would be the challenge if we want to use your approach on the non-oriented graph ?

  The graph is similar to a non-oriented graph, as all edges are 'duplicated' such that for an oriented edge connecting vertex 1 to vertex 2, and oriented edge connecting vertex 2 to vertex 1 exists. We use oriented edged as a way to integrate general flow information such as the main flow direction. This clarification will be added to section 2.2.1 at the revision of the manuscript.

Details

- **Formulas and equations**

In most of the paper formulas and equations one or two terms are not defined in the text. It is quite easy to guess who is who, but it is not homogeneous. You can whether pass through all variables and all texte in the article or create a table of annotations in the beginning of the Method paragraph.

We will carefully check that at the revision of the manuscript.

- **2.1 Experimental settings:**

In real study, if the transmissivity of the fault is unknwon, one would define an uncertainty range as a continuous random variable. Would your approach work in this case ? Or, because of the efficiency, discussed earlier for the homogeneous media, there are some intermediate situations where it would not work and though would not discriminate the multiple generated cases?

The sensitivity of uncertainty range around fault transmissivity could be tested. But it is likely that in some intermediate situations, the ambiguity would remain and the proxy would not enable to discriminate between different cases. However, such a sensitivity analysis can be solely conducted on the proxy (without running a physical solver), by looking at the sensitivity of different fault transmissivity values on the shortest paths or graph distance maps; it could then be used to define range of values for differentiable scenarios.

- **2.2.1 Graph generation:**

[99] Figure 2. There is a figure of the conventional grid containing a 3D property. This paragraph is focusing on the graph creation. May you illustrate the resulting graph ? or at least a zoom on the peace of the graph ?

Given that the graph connects each neighbouring grid cell, it would not identify specific features and not simplify the visualization of the model for the reader, thus we chose not to provide such a plot.

[100] Equation 2. Variables R hydraulic and *dl* are not referenced.

R is the hydraulic resistance and *dl* is the incremental length along the path. As mentioned earlier, we will carefully check that the variables and notations are properly defined at the revision of the manuscript.

[106] Equation3. Variable Re is not referenced. …

R_e is the hydraulic resistance of edge *e*. As mentioned earlier, we will carefully check that the variables and notations are properly defined at the revision of the manuscript.