Reply to Reviewer #1

We would like to thank the reviewer for his comments and suggestions. Below please find our detailed response to the reviewer's concerns.

In this case the title says it all, or almost... I was quite thrilled when I read the title and introduction since I was expecting to see an application of the EnKF to a realistic case (port-Rotterdam inspired), unfortunately the final outcome is a nicely written, quite interesting analysis of the efficiency of the hybrid and the exact second-order sampling formulations of the EnKF, but the application, although port-Rotterdam-inspired, is far from being realistic at all. And the authors fail to recognize it.
The authors make no comment about the statement in line 345 "Modelling parameters required for running the coupled FTR-Model, such as porosity, distribution coefficients and others are defined, based on real data and laboratory assessment, as 3D heterogeneous fields" (They forgot to mention explicitly hydraulic conductivity.)
This assumption means that all the uncertainty associated with the heterogeneous geological parameters is discarded, and that all the analysis has been performed assuming that porosity, conductivity, distribution coefficient, and other parameters are perfectly known. Once this is realized, one has to continue reading under the understanding that what follows is a purely academic exercise, poorly disguised as a realistic application.
The authors must be very clear from the very beginning on this "small" detail, and acknowledge it. Apart from that, I think the paper is well written, hard to follow at times, and provides an interesting discussion on how to deal with the specifics of the hybrid and the exact second-order sampling formulations of the EnKF.

The reviewer raises a good point. Improving the estimates of the groundwater flow, on top of the contaminant dynamics (transport & reactions), is rather important. This is usually done, as the reviewer points out, by quantifying the uncertainties of the hydraulic parameters such as conductivity and porosity. This has been extensively studied in the Hydrology literature.
Our focus in this paper, however, is to address two major drawbacks of the EnKF; namely the forecast under-sampling and observation sampling errors. We present this while focusing on a slightly different, but related, application and that is quantifying the uncertainties associated with subsurface biodegradation reactions. To the best of our knowledge, this would be the first application in which biodegradation parameters are estimated in a near-realistic modeling scenario using the EnKF. Addressing the uncertainties of subsurface hydraulic parameters is possible but is beyond the scope of the current study. Following the reviewer's suggestion, we now clarify this detail in the introduction section. The reviewer may refer to lines 99-101.
Concerning line 345, we now provide more details on the offline procedure we follow to estimate the hydraulic properties of the subsurface such as porosity and conductivity. In essence, the hydraulic conductivity is provided in the database GeoTOP. The GeoTOP for the province of South-Holland is constructed using 46.000 borehole data. Using the borehole data, the most probable lithostratigraphy and lithofacies have been estimated in each voxel of 100x100x0.5 m. The GeoTOP further uses relations between the lithostratigraphical units and the lithofacies with parameters such as hydraulic conductivity, porosity and organic carbon content in order to provide these parameters on the voxel scale. Further details and essential referencing are provided towards the end of Section **3.2.2**.

Minor comments

Line 129: What do you mean by "...the EnKF computes an approximation of the joint pdf..." Unless you mean the non-parametric joint pdf as implied by the raw set of ensemble values, the statement is incorrect. The EnKF is based on means and covariances, but this does not imply that by knowing them you know the joint pdf.

Given the limited ensemble size, we refer to the joint pdf suggested by the EnKF at every forecast step as an approximation of the "true" pdf. We agree with the reviewer, having the mean and the covariance does not necessarily give us access to the entire true distribution of both state and parameters. This was made clearer in the revised text.

Line 160. There is no Gaussian assumption in the derivation of the Kalman filter equations!! Those equations are solely based on means and covariances and there is no requirement that parameters or state variables are Gaussian to derive them. However, it is true that the EnKF is optimal for multiGaussian-based variables.

By construction, the Kalman Filter accounts only for the first and second moments of the estimated random variable (state or parameters). When the pdfs are not Gaussian, it is only optimal along linear estimators and when both the model and observational operators are linear. As the reviewer suggests, when the distribution of the unknowns is multiGaussian (and the model is linear) the EnKF is optimal (for an infinite ensemble size). This is however almost never the case when parameters are also part of the state vector, as in the case of our study. The sentence was revised to remove any confusion.

Line 483. ... the "famous" steady-state Kalman filter... Please, watch your wording and avoid sensationalism.

The word famous has been removed. Thank you.