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Discussions

Interactive comment on "On the efficiency of the hybrid and the exact second-order sampling formulations of the EnKF: A reality-inspired 3D test case for estimating biodegradation rates of chlorinated hydrocarbons at the port of Rotterdam" *by* M. E. Gharamti et al.

Anonymous Referee #3

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In the paper by Gharamti et al., the authors compare three data assimilation strategies for a subsurface state-parameter estimation problem: the standard ensemble Kalman filter (EnKF), a hybrid EnKF including optimal interpolation (EnKF-OI) and a second-order sampling formulation of EnKF (EnKF-ESOS). Synthetic data assimilation experiments are performed with a reactive transport problem for migration, sorption an degradation of chlorinated hydrocarbons. This set-up should mimic a contaminated aquifer in the port of Rotterdam. Concentration data and first-order degradation rates are up-

dated within the three assimilation schemes.

The paper is well written and points out important limitations of the ensemble Kalman filter in subsurface characterization (undersampling of forecast covariances and observation errors) and how they could be ameliorated with EnKF-IO and EnKF-ESOS. However, I have two major concerns regarding the content of the paper:

(I) It seems to me that there is a considerable overlap with earlier work from Gharamti et al. (2014). Large parts of the paper related to the EnKF-OI contain very similar information as in the earlier work and also the overall model set-up is quite similar in both studies (see below) leading to almost the same conclusions regarding EnKF-OI. Therefore, the authors should give a clear motivation why the comparison EnKF/EnKF-OI is repeated in this paper and they should point out what is the innovative aspect of this study compared to their previous work (i.e., what did we learn from this study regarding EnKF/EnKF-OI that was not already covered in Gharamti et al., 2014).

(II) The authors claim to use a 'reality-inspired' test case for the comparison of the different data assimilation schemes. In fact, only a limited amount of information about the site characterization is given in section 3.1 which makes it difficult for the reader to judge how realistic the model set-up is. For example, how many measurements were available to derive the parameter fields for hydraulic conductivity, porosity and distribution coefficients and how uncertain are the derived parameter fields? Is the model discretization fine enough to account for the spatial variability of subsurface parameters? Another question is whether the assumption of steady state groundwater flow is valid for the chosen site. Usually, one would expect transient groundwater flow due to temporally variable recharge, pumping activities or density-driven flow in such environments. Transient groundwater flow could have important implications for the data assimilation, e.g., for the determination of the background covariance matrix in the EnKF-OI scheme (see below). Overall, the current set-up is very similar to what has been used in Gharamti et al. (2014) except that groundwater flow is 3D in this example (which should not be a major issue when a steady state flow field is used) and the chemical reactions are different (but follow a very similar mathematical description). So in fact, I think that there is not much more complexity in this 'reality inspired' set-up than in the 'purely' synthetic set-up used in previous studies. Therefore, I suggest the authors to add more complexity in their model set-up in order to test the different assimilation schemes under more realistic conditions. This could be accomplished e.g., by considering more sources of uncertainty (e.g. hydraulic parameters, forcing terms) and by using transient flow conditions.

Specific comments

Line 191-192: The same applies for the alpha and beta values in EnKF-OI.

Line 195-196: What do you mean with '...dynamically constants quantities....'?

Line 216-217: Incomplete sentence.

Line 368-370 and Figure 5: Why does PCE appear in layer 40, when the contaminant source is located in layer 60 and the pre-dominant flow direction is downward? Is the groundwater flow rate so low compared to molecular diffusion?

Line 396-417: In this example, the background covariance matrix for EnKF-OI is derived on the basis of a steady-state flow field with perfectly known hydraulic parameters. Additionally, the background covariances are derived from the same time period, where the assimilation experiments are performed. This means that the derived background covariance matrix contains a very precise description of the relation between concentrations and degradation rates in your system. However, under real-world conditions the uncertainties in hydraulic parameters may have a considerable impact on the quality of the background covariance matrix. Additionally, under transient flow conditions it might be much more difficult to derive a good estimate of the background covariance matrix. Therefore, I suggest the authors to discuss such practical issues in more detail and also to perform additional simulation experiments where these influences on the derivation of the background covariance matrix are assessed in more detail, e.g. by

introducing uncertainty in the hydraulic parameters and by using transient flow conditions. This would provide a more realistic assessment of the EnKF-OI assimilation scheme.

Figure 11: It would be helpful in this plot to also show the evolution of concentration values without data assimilation as a comparison. Additionally, why does the optimized EnKF-OI simulation (grey lines) for PCE update in the wrong direction between year 5 and 10?

References

Gharamti, M., Valstar, J., Hoheit, I. (2014): An adaptive hybrid EnKF-OI scheme for efficient state-parameter estimation for reactive contaminant transport models, Advances in Water Resources, 71, 1-15.

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