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Interactive comment on "On the Conceptual Complexity of Non-Point Source Management: Impact of Spatial Variability" *by* Christopher Vincent Henri et al.

Anonymous Referee #2

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The present work deals with the feasibility of simplify the conceptual modelling of non-point source (NPS) contamination of an aquifer, in the presence of an active pumping well. The simplification consists of spatial homogenization of otherwise heterogeneous terms (recharge rate and contaminant concentration of the recharging water) and of the aquifer hydraulic properties (conductivity). I liked the general goal/purpose of the study (even though there is no theoretical/technical novelty in the employed methodology) and its practically oriented nature. Nevertheless, it is my opinion that there are several unclear points and unstained observations that should be addressed before acceptance for HESS. I list my concerns below. I do see a very good paper after addressing these issues/confusions. I also hope that my comments help in making the

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paper shorter and clearer, it becomes quite hard to follow it from the beginning to the end.

Line 5-9: ‘On the other hand, concentration levels of some key NPS contaminants (salinity, nitrate) vary within a limited range (<2 orders of magnitude); and significant mixing occurs across the aquifer profile along the most critical compliance surface: drinking water wells with their extended vertical screen length. Here, we investigate, whether these two unique NPS contamination conditions reduce uncertainty such that simplified spatiotemporal representation of recharge and contaminant leakage rates and of hydraulic conductivity are justified when modeling NPS pollution.’ I don’t agree with the fact that the Authors tested that the two mentioned conditions imply a reduction in the uncertainty (they do not explore scenarios where these two conditions aren’t meet!). I would say that the Authors investigate, under these two peculiar NPS conditions, the possibility of introducing simplifying modelling hypotheses which do or do not affect the ensuing uncertainty about targeted quantity. Please consider revise the sentence, here and throughout the whole paper where needed.

Line 14-15: ‘Surprisingly, regional statistics of well concentration time series are fairly well reproduced by a series of equivalent homogeneous aquifers, highlighting the role of NPS solute mixing along well screens.’ I have two comments here: (i) the term regional statics is somewhat obscure; (ii) once clarify it in the section 6 (see also my comment 3), it is my understanding that the diverse homogenization here proposed work fine for low (i.e., 0.1) and middle (i.e.,0.5) probability of exceeding a given concentration in the well, while for high probability (i.e., 0.9) the homogenization-based results are unreliable (see e.g., the discrepancy between the curves in Figure 6a and Figure 10a, in Fig. 10a I don’t see the ‘regional’ counterpart (red dashed curve)).

Lines 90-92: ‘Assuming ergodicity (Dagan, 1990), stochastic management metrics are quantified both, for the pollution variability across an ensemble of production wells encountered over a basin, and for the uncertainty about pollution levels at an individual well.’ As a matter of fact the Author verified the validity of the ergodicity principle (here in the sense that the results of one single realization are representative of the results across the whole ensemble of realizations, or, in other words, there is no variability across the ensemble of realizations of the investigated output) only with respect to the soil crop arrangement (see Fig. 1), but ergodicity does not hold with respect to the (either heterogeneous or homogenized) aquifer conductivity (i.e., their results clearly show that there is a variability in the investigated NPS management metrics as the conductivity distribution varies among realizations)! Please clarify this point. The Authors named the regional analysis ('pollution variability across an ensemble of production wells encountered over a basin') (see also Section 6) the scenario in which both the conductivity and the land crop usage varies between the Monte Carlo simulations. They referred to the single well analysis ('uncertainty about pollution levels at an individual well') when only the conductivity varies among the MC simulations (with the crop arrangement fixed). To me this distinction is not meaningful, since it implies that in the groundwater basin there are sub-portion (the simulated domain) subjected to the very same boundary conditions (aside from the infiltration rate) and that these sub-portions do not influence each other (they are far away from one another). In my vision the Authors have, given a domain of interest and deterministic initial and boundary conditions (aside from the infiltration rate), conducted the uncertainty analysis (i) for a given (i.e., conditional) to a crop arrangement and (ii) considering the uncertainty in the crop arrangement, proven then that the uncertainty in the latter is not an influential factor (i.e., there is ergodicity w.r.t. to the crop usage). Please consider this aspect, the regional and one-well distinction seems to me confusing and not well supported by the investigated set-up.

Line 115-117: 'Assuming ergodicity (Dagan, 1990), stochastic analysis is applied to first quantify uncertainty about pollution outcomes at individual wells and to secondly quantify regional spatial variability in pollution outcomes across an ensemble of wells'. Please revise this sentence according with Comment 2-3. Furthermore, in the way it is written it means that ergodicity is needed in order to quantify uncertainty (this is the case for example in geostatistical approach where spatially distributed measure of conductivity in a field, i.e., in a single realization, are employed to describe the ensemble statistic of conductivity) in this study, i.e., that automatically a single realization is sufficient to describe the behavior of the ensemble, whereas, it is my understanding that the Author did the other way around: prove the validity of ergodicity (for the investigated quantity) w.r.t. to the crop usage. If ergodicity was originally assumed, no need to do many simulations.

Line 129-130: 'The histograms of the mean and the variance of the logarithm of K are shown in Figure SM3. Fifty realizations were sufficient to converge the lower statistical moments of K and of the resulting mean velocities (Figure SM7)'. It is not clear at all that the Authors are referring to the spatial mean and spatial variance (this is my impression) evaluated for each field of K, and then doing the histogram of these quantity.Is it so? Why do we care about it? How do the Author prove the convergence of these spatial mean and spatial variance employing 50 realizations? To which values should these quantities converge? I am way more concerned about: are the 50 realizations enough to ensure the convergence of the statistics (e.g., pdf, CDF) of the output quantities of interest (i.e., travel time, breakthrough curves at the well and capture zone)? This is aspect is not investigated at all by the Authors and looking to the high spatial variance of K (from 10 to 18 approximately) I am afraid that 50 realizations are not enough, even if the source is spatially distributed. Please analyze the convergence of the investigated results w.r.t. to the Monte Carlo simulations. Furthermore, regarding the histogram in SM3 and SM4 for the recharge rate and the concentration of pollutant in the recharge, why do we care about them? Please clarify.

Line 151-195: I see the detailed description of the estimation of the recharge rate to better fit in an Appendix.

Line 230-233: 'The detailed discretization of the velocity field described above is capturing the most relevant characteristics affecting the macro-dispersive transport behavior (LaBolle, 1999; LaBolle and Fogg, 2001; Weissmann et al., 2002; Henri and Harter,2019). Therefore, effects of grid-scale dispersion are assumed to be negligible.'

So, does the Author set the tensor D in (10) equal to zero? Please clarify.

Line 244-246: 'Three relevant nonpoint source (NPS) pollution management metrics are considered to measure the stochastic simulation outcomes: the probability distribution of pollutant travel times to wells, the probability distribution of pollutant concentration in wells, and the probability distribution of source locations.' These are the 3 quantities of interest, why do you introduce them in the 2.3.1 Pollutant travel times section? Better just before.

Line 250-251: 'Following a stochastic approach, probability density functions (pdfs) of travel times ti are obtained by determining the histogram of ti in 150 simulated wells'. Please note that the histogram is not a pdf, whereas the latter is associated with a continuous variable and the former to a discrete variable. I would limit to say to that the pdf are estimated on top of the 150 simulated wells. Furthermore, at lines 244-246 the probability distribution is mentioned, this is not the pdf. Also, at line 214 the authors say that they analyzed the probability distribution, but then in Figure 3 they depict the pdf. Please check for the consistency of the terminology/results through all the work.

Lines 262-263: 'NPS pollution management may also require the assessment of the effective source area, i.e., the capture zone or contributing area of the pollution observed in a production well.' Please avoid to use source zone, this is typically used to indicate the area covered by the contaminant at the initial time (regardless if it reach the well or not), the capture zone of the well is way more clear as the wording in my opinion.

Line 275-277: 'The NPS metrics from fully heterogeneous simulations are compared to the NPS metrics obtained from a range of upscaled, homogenized simulations that employ effective homogeneous properties rather than the original heterogeneous distribution of the K, r, and c0 terms'. Please consider avoiding the word upscale/upscaling (here and in the whole text), since this inherently implies a change of scale (e.g., from pore to continuum or from continuum to continuum) and it is typically associated with a change of the governing equations used to describe the process (e.g., effective model for the solute transport involving non-local terms) whereas here the Author conducted a simple homogenization (with the arithmetic average as a rule) of the diverse terms.

Line 286-292: 'To simulate flow and transport in an equivalent homogeneous, upscaled K conditions, we estimate the effective longitudinal and transverse vertical hydraulic conductivity, K*x and K*z , and dispersion, alpha*L and alpha*T. Effective parameters in the longitudinal direction (K*x and alpha*L) are determined from the first and second spatial moments of a plume resulting from an injection of mass in a vertical plane of width 3000.0 m and depth 50.0 m. The same approach is adopted to estimate the effective parameters in the transverse vertical direction (K*z and alpha*T) by injecting particles in a horizontal plane covering the entire top of the domain. No extraction is considered in both cases in order to capture the natural behavior of the plume.' What about the K*y and dispersivity in the y direction? Furthermore, 'No extraction is considered in both cases in order to capture the natural behavior of the plume', but the ensuing macro-dispersion of a plume is influenced by the presence of pumping well (e.g., radial versus uniform flow conditions), please clarify/justify this aspect.

Lines 317-316: 'For all simulations, early mass travel times are within a range of 10 to 100 years with an expected value (highest probability) of 50 years (Figure 3a).' For a continuous variable is not possible to define the value with the highest probability (it is possible for a discrete variable). Furthermore, the expected value of a pdf does not always coincide with the value where the value of the pdf is the highest. Clarify.

Lines 346-347: 'Spatial variability in the recharge is responsible for somewhat more uncertainty in the exact delineation of the capture zone along its margins than what is captured by the homogenization of r.' Is not r the symbol to indicate the recharge? I think r should be replaced with C0 or vice-versa. Furthermore, focusing on the impact of the homogenization of the recharge (compare Fig. 4a with Fig. 4c) I would say that the homogenization of the latter is associated with a less spatially extended capture zone w.r.t. to the case in which the recharge is treated as heterogeneous, this does

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not mean that the there is more uncertainty in the delineation of the capture zone. Furthermore, looking to the Fig. 4 I would say that capture zone is not well-delineated along its border, due to the low number of Monte Carlo realizations. Please check it and revise the sentence.

Lines 379-380: ‘For an individual well, the results indicate that there is a 10% chance for nitrate concentrations to start to rise before 30 years, a 50% chance to rise no later than 50 years, and a 90% chance to rise before 70 years’. Should not be after X years?

Lines 402-404: ‘Homogenizing only concentration also leads to an underprediction, by about 20%, of concentrations exceeded by either 90%, 50%, or 10% of well, relative to the fully stochastic land use treatment (green lines in Figure 6).’ Is green correct?

Lines 471-472: ‘ . . . only adds a moderate degree of uncertainty to the capture zone delineation..’ see Comment 15.

Line 480: ‘The observed gradient of travel times’ I don’t see any gradient (i.e., âĹĞ) of the travel times evaluated by the Authors. There is a spatial variation of the mean travel time in Fig. 9, but this is different from a proper evaluation of the gradient. Please revise the sentence

Lines 487-489: ‘Thus, contaminant mass reaching the top of the well has little variability – here only to the degree that the homogenization is done individually for each realization, leading to some minor variability in the homogenized K between realizations.’ Why does the fact that the mass reaching the top of the well exhibits a low variability (note that the Authors do not provide a quantification of it) lead to have minor variability in the homogenized K? Please clarify.

Lines 489-491: ‘More uncertainty is observed on the upstream side of the capture zone since it represents mass reaching the bottom of the screen, the vertical position of which is realization dependent’ I suppose this comment is related to Fig. 9, which depicts the expected value of the travel time to the well. The latter gradually increases as we move upstream w.r.t. to the well location. I don't see this as a measure of an increasing level of uncertainty! It could be that the expected value of the travel time increases, but it can also be that spread (e.g., measured through the variance) of the pdf decreases. Please consider evaluating at least the variance of the pdf of travel times as a quantification of the degree of uncertainty.

Lines 520-521: 'Results show that homogenized K-fields perform more poorly to predict the lowest concentrations (P90) than the highest ones (P50 and P10).' Why P90 is associated with low concentrations? P90 is a probability, looking at Fig. 10a I see that for a given concentration (either high or low) there is a time necessary to exceed this level of concentration in the well with a probability of 0.9. The way I interpret Fig. 10 is that homogenized solutions are in good agreement with the heterogeneous case, when it is a matter of evaluating low (P10) and middle (P50) probability of exceedance of a given concentration, but the homogenized solutions do not work well for high (P90) probability of exceedance of whatever concentration.

Conclusion: I note a change of style in the conclusion, whereas there is a more consistent and proper use of the terminology with respect to the rest of the work.

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