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Interactive comment on "Estimation of effective porosity in large-scale groundwater models by combining particle tracking, auto-calibration and ^{14}C dating" *by* Rena Meyer et al.

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General comments

The paper details a significant modeling effort demonstrating the importance of carbon-14 dating in the calibration of spatially-distributed porosity. The study utilizes a previously calibrated 3D groundwater flow model of the site and selects 11 of 18 carbon-14 data as targets. I have two major concerns and several other concerns about the implementation of the inverse method and the conceptualization of the apparent ages. The latter are detailed in the specific comments and the former are: 1. the model assumes the conductivity field inherited from the (unpublished, at the time of this review) Meyer et al. (2018a, and b which is in preparation); and 2. the data are prefiltered (e.g., eliminated) based on their coherence with the inherited model prior to the analyses. While I highly respect the authors' work in the field and I believe this work has a substantive contribution in the rarely touched world of porosity estimation, I think there are important elements that require consideration and careful address in the discussion. Details of my concerns follow.

The very significant reliance on the unpublished groundwater flow model, and its fixed hydraulic conductivities, raises concerns about the current study. The current study seeks to identify porosities of 7 geological units by fitting them so that the mean ("direct") ages match the apparent ages from carbon-14 corrected for dissolution and diffusion; however, there is no allowance for departures from the originally calibrated conductivities (from the unpublished Meyer et al. 2018a). Thus the porosities are treated as if they are independent of the hydraulic conductivities. This is not conventional and disagrees with current understanding of the properties of natural porous media, and needs to be addressed by the authors.

Multiple aspects of the inversion done in Meyer et al. are important here since that work laid the foundation flow model; for instance, the vertical anisotropy factors assigned from that work are 25 for sand and 85 for clay units, which are quite high, and qualitatively at least would seem to restrict vertical migration of water in a way that would definitely affect age.

A more robust approach would have been to do a wholistic inversion, where the conductivity (and other flow and transport parameters) were calibrated at the same time as the porosity (and other transport parameters, including the dispersivity, set to zero here based on a brief local sensitivity), to the collective head and apparent age data. Why this is not done, and the potential constraints on the resulting two-stage inverse, should be discussed. There are no error plots from the prior head-inversion of Meyer et al so the success of the calibration of the flow equation is unknown. More importantly for a subsquent inversion for porosity, there is no indication of the uniqueness of that

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first inversion. Even if that inversion gave good results, it may be nonunique, and it seems that there may be a different set of hydraulic conductivities and porosities which together might fit both the available head and carbon-14 data.

The elimination of dispersivity appears not only somewhat arbitrary but also contradictory to the authors' overall argument for the importance of porosity (cf. specific comment on page 8 line 21). It appears they have replaced the modeling of mobile-immobile domain mass transfer in the model with the approximate diffusion-correction applied to the data. This could be justified based on pragmatic grounds but the discussion in this regard is lacking. The alternative to use effective mobile-immobile domain mass transfer seems potentially useful and pragmatic as well but is not discussed.

Very important is the unsupported elimination of 7 pesky carbon-14 data (cf specific comment on page 8 line 30). The focus only on the data which are consistent with the already partly calibrated model brings the entire study into question.

Why the recently developed methods for full distribution of age (e.g., several articles in J Hydrology, December 2016) are not used is not described; however, this may be attributed to the reliance on single radiometric tracer (carbon-14) concentration measurements, which precludes any inferrence of age distribution.

Specific comments.

page 2 line 4. "Three different apporaches with specific benefits and disadvantages are commonly applied to simulate groundwater age..." The given list of commonly-used methods is not complete (there are also the lumped-parameter approach, and the mixing cell model approach), and equally important are the new methods which are generally more robust [solving the actual equation of groundwater age, either by the Laplace method of Cornaton (WRR 2012) or by using reduced dimensions as in Woolfenden and Ginn (Groundwater, 2009)]. The review by Turnadge and Smerdon (J Hydrology 2014) provides a more complete listing and assessment.

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page 2 line 12. "A comparison of ages simulated using any of these methods with ages determined from tracer observations, referred to as apparent ages is desireable..." This is true but omits the very important point that "ages determined from tracer observations" are not equal to mean ages, especially as in the present case of decaying environmental tracers (e.g., carbon-14). The rest of this paragraph summarizes part of the way that "apparent ages" are misled by old carbonate dissolution, by diffusion, and by heterogeneity, following McCallum's work; however, it should also point out the fundamental difference between mean ages and radiometric ages described explicitly by equation 16 of Varni and Carerra (WRR 1998), and the general relation between distribution of age and the radiometric age given in Massoudieh and Ginn (WRR 2011).

page 2 line 238. "Bethke and Johnson (2002) concldued that the groundwater age exchange... is only a function of the volume of stored water." This is misleading because it is valid only for the mean groundwater age, and requires steady-state as detailed in Ginn et al. (Tranpsort in Porous Media, 2009). Also this point is made earlier and more precisely in Varni and Carerra (op. cit., page 3272), who points out that it is actually a result of Haggerty. The overall point by the authors that porosity is important to age modeling is valid.

page 3 line 1. "neglecting dispersion effects seemed to be acceptable at large scale" is unsupported for the present application, results of cited Sanford and later Gelhar notwithstanding. See comments below (re: page 8 line 21 and the reliance on Sanford; page 10 lines 14-17 and Figure 8) for more discussion.

page 6 line 27. "Meyer et al. (2018b) simulated ....further details can be found in Meyer et al. (2018a)." Actually they cannot because Meyer et al. (2018a) is in submitted state (page 30 line 28). This is quite important because the present authors have chosen to rely upon the hydraulic conductivity field previously calibrated in that work, and here do not allow the conductivity values to be modified in the inversion using carbon-14 inferred ages (page 8 line 26).

page 8 line 2. "The resulting head distribution is shown in Figure 1." Figure 1 shows (it seems to me) only the shallow aquifer heads. It is well-known that the quality of an inversion of the flow equation (to determine hydraulic conductivities) depends on a broad spatial distribution of the heads, and it is unclear that such head data were available to Meyer et al. Also, there are no error plots showing the goodness-of-fit of the flow inversion to the measured heads, so it is impossible for the reader to evaluate how good was the flow equation inversion. Also it is impossible for the reader to evaluate the uniqueness of the flow equation inversion, which is commonly very poor.

page 8 line 21 "According to Sanford (2011), neglecting hydrodynamic dispersion... on a regional scale is a reasonable approach when old-age tracers, such as carbon-14, are used as dispersion might not be crucial for these tracers." This sentiment is unclear because it suggests that there is something particular to the carbon molecule that frees it from dispersion, which is quite incorrect. It is also directly in opposition with the authors' claim (page 2 line 28ff) that porosity is important for groundwater mean age determination because "groundwater age exchange between flow and stagnant zones is only a function of the volume of stored water."

page 8 line 30ff. The authors removed 7 data from their 18 carbon-14 measurements becaue the values did not match their conceptual model; 6 were deleted because the carbon-14 activities were below 5pmc, and one due to proximity to another sample with different value. The justification given for the first 6 is "it was assumed that the boundary conditions of the flow model ... were not representative for pre-Holocene conditions." This justification is unclear at best; the model is steady state so the initial conditions do not matter, and the boundary conditions are necessarily (by the steady-state assumption) constant. Thus the elimination of the low carbon data is unsupported. The elimination of the 7th datum is only weakly justified, as there appears to be nothing wrong with it other than its troubling value.

page 9 line 4-6. The weights on the data used in the inversion were all the same. They were based on an average uncertainly of apparent ages of $\sim$102 years, as per "average

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of the standard deviation of the diffusion correction for the selected 11 samples..." This defeats the purpose of calculating individual standard deviations for individual data in the first place. The individual standard deviations (Table 1, last column) show a range of 8 to 310 years, so individual weights based on these values would have led to significantly different weights. Individualized weighting is rarely possible in groundwater flow model inversion but is often possible in transport inversion, and it seems to me that the authors have unintentionally limited the inversion by assigning equal weights to all apparent age data. The importance and utility of weighting is amply described in the books by John Doherty and Mary Hill, and could have been used to condition the data per their individual certainties; moreover it could have been used to condition - perhaps to good end - the pesky 7 data that were eliminated instead. In fact, the standard deviations of the 6 eliminated data range from 1323 to 2593 years, which would have led to quite significant reduction in the importance of these data as the weights are generally taken as the reciprocals.

page 9 line 27. "mean groundwater age is simulated in analogy to solute transport as an "age mass" (Bethke and Johnson 2008)." This "age mass" requires mathematical and physical definition; as pointed out in Ginn et al (2009, op. cit., section 2.2) the definitions of Goode and of Bethke and Johnson are not clear or consistent. The example of Bethke and Johnson involves an aquifer and an aquiclude with only immobile water, so that diffusion is the only mechanism by which exchange can take place. If it is eliminated, then the argument collapses.

page 10 lines 14-17 The numerical experiments to evaluate dispersion effects, described here, with results summarized on page 15 lines 10ff and in Figure 8, are apparently done on one model, that is, on one assignment of hydraulic conductivities and porosities. It is not clear which porosities were used. In any case, this is at best a local parameter sensitivity analysis and it would be more accurate to include the dispersivity values in the inversion. The argument that the 200mx200m grid cell size is sufficiently resolved to allow ignoring dispersion is unconvincing, because there are multiple mod-

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eling exercises where the effective dispersivity is proportional to the grid cell size, not zero. Figure 8 does not tell how the errors grew but only the total error - did the errors go biased ? If one were to guess, I would bet they did, because the dispersion would allow mass transfer laterally, causing generally older ages.

page 11 line 6 "...as porosity does not impact the trajectory of the particle path..." this is true only via the assumption that the porosity and hydraulic conductivity are independent, which is not common.

page 13 Figure 4a. The plot demonstrates in my view limited improvement for two reasons. First, the 5 older water samples (with carbon-14 corrected ages greater than 500 years) show significantly improved fitting in 3 cases, with one getting worse. Second, the plot is absent of confidence intervals (compare for instance to Figure 11) which could be it seems to me estimated based on the standard deviations of the corrected carbon-14 ages (Table 1), with additional uncertainty based on equation 16 of Varni and Carrera (op. cit.). The recognized uncertainty in the apparent ages should it seems be used to condition the results of Figure 4a.

page 16 line 4ff "Hence, the dispersivity only describes the effect of heterogeneity at the grid scale, 200m. In accordance with Gelhar et al. (1992) this results in (dispersivity) with a magnitude of a few meters." I am unaware that Gelhar suggested this dispersivity value given (only) the size of the grid, please provide the page. Also in the intervening 25 years there has been extensive research and articles on the effective dispersivity for regional groundwater models, and more up to date referencing is called for. Notably, the model (including its effective parameters) at the 200m grid block scale tells only the expected or mean concentration in the grid block, that is, the concentration in the model is treated as a constant on the 200m x 200m x 5m grid block, while the carbon-14 data are collected from sampling wells on much smaller spatial scales - this issues should also be addressed or at least noted.

page 17 line 1. "The age distribution is strongly affected by geology and is therefore in good agreement with the interpretation of the flow system by Meyer et al. (2018)." This statement is unclear: the age distribution is always strongly affected by geology.

Figure 10 caption "Normalized probability distributions..." These are frequency distributions becasue there is no randomness in the model or its parameters.

page 21 line 12 (regarding Figure 11) "However, most of them lie within one standard deviation." Seven of the standard deviations here span several thousands of years while the means for all but one are less than 7000 years, so this is not a comforting result.

page 23 section 5.1.2. This discussion clearly identifies the ways that individual particle path history of exposure to different geologic units differentiates the actual true correction of the carbon-14 from the simplified correction done in the paper; however, it still does not tell about the fundamental difference between the apparent age and the mean age (cf. comment on page 2 line 12). That is, even if the correction were perfect, the apparent age would not equal the mean age.

page 24 line 6. "While direct age corresponds to the flux-averaged mean, the particle tracking age is resident-averaged (Varni and Carrera, 1998)." I do not see where this statement is given in the cited reference, please clarify if so; furthermore, I do not believe the statement is correct. The mean age of the model of Goode is an Eulerian quantity, just like a solute resident concentration. The relation between resident and flux-averaged concentrations is given in a number of papers by Parker and van Genuchten and coworkers (1984) but the governing equations that result are mainly restricted to 1D cases.

page 24 line 9. The use of harmonic mean for particle ages is absent of a rational basis other than it seems to fit the data well, and a generic reference to Konikow (2008). The specific manner of averaging the particle ages should be physically-based and independent of how well it fits the data in a particular setting.

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