The authors investigate the groundwater flow system, the heat and mass transport processes along a two-dimensional model of a high-energy subterranean estuary. During a year and a half of field observations — with sampling varying in time and space — they recorded the hydraulic head, temperature, salinity, and water age. A significant part of the model parameters (49 in total!) was determined by calibration, performing approximately 10,000 simulations and "selecting the best solution" using the particle swarm optimization (PSO) method. I consider the work performed to be very enormous, the techniques used (field measurements, numerical simulation, automated calibration) to be very comprehensive, and the results achieved and presented to be realistic. In light of all this, I consider the manuscript — after some clarification and completion — suitable for publication in the HESS journal.

Major comments/concerns

1. The description of the numerical model is rather sporadic, which does not facilitate the work of modelers, a deeper understanding of the article, or its potential reproducibility. Therefore, I suggest:
    a. the equations used in the simulations should be presented in the article if possible, or at least in the supplementary material, where it should be clarified that water density depends purely on concentration, while viscosity is constant.
    b. Due to the complexity of the processes, the boundary conditions are also very complicated (Section 2.2) and difficult to follow. It would be useful for the reader if they were summarized in a figure, emphasizing their time dependence. This would also be useful because the total length of the model is 1450 m (Page5Line134), but the entire model area is never shown in the manuscript, only between 500–1300 m and 800–1300 m. This would also eliminate the shortcoming that I could not find any information on the salinity, temperature, and water age boundary conditions for the vertical and lower boundaries.
    c. Fixed model parameters (e.g. R, S_s, D) should be tabled too.
2. The PSO algorithm is indeed suitable for finding the minimum of highly non-linear inversion problems, although this is a major challenge in the case of a model involving almost 50 unknowns, time-dependent, free topohaline convection. Could you show a figure that illustrates the convergence of the method? What object function did PSO use to quantify the individual simulations at the pilot points?
3. The cross plots in Figure 3 show the relation between the measured data and the simulated results for different calibration quantities. The figure is not discussed in the manuscript, which could answer some of the arising questions. Are the parameters of the best-fitting model shown on the y-axes? Were these diagrams used by PSO to qualify each simulation? Are the quantities at different pilot points and at different times shown here? Are all measurement points given equal weight? Could this explain why the root mean square error of the smaller number of water age data is much greater than that of the large number of e.g. head data? I would appreciate an explaining paragraph regarding Figure 3.
4. The thermal retardation factor was fixed during the simulations, R=2. This value seems very high, although there is some ambiguity in the literature concerning the definition of the R value. What porosity, density and specific heat values give this factor?

Minor comments

Fig. 2 It would be useful to indicate the north-south direction.
P7L181 Dez → Dec
P15L326 ^{3}He → ^{3}H

P15L332 $^{3}He \rightarrow {}^{3}H$

P16L362 permeable material → permeable medium/sediment…

Fig. 7 caption I guess the figure illustrates the standard deviation of simulated salinity, groundwater age and temperature time series along…

P17L382 Figure 5 → Figure 5.b

P20L457 Reference is missing

P20L460 Reference is missing

It is somewhat surprising that the terms “biogeochemical” and “reactive” appear 16 and 11 times in the manuscript, resp., even though the simulation does not involve biogeochemical or reactive transport modeling...

Overall, the work presented in the manuscript is very substantial, multifaceted, and fits well with the subject matter of the HESS journal, so, after taking into account the above clarifications, I support its publication.