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Geoscientific Model Development Discussions

Interactive comment on "HydroMix v1.0: a new Bayesian mixing framework for attributing uncertain hydrological sources" *by* Harsh Beria et al.

Anonymous Referee #1

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General comments

The discussed paper is well written and follows a clear and logical structure. Mixing problems are an important area of research and potentially relevant for many applications, which is why the manuscript is of potential interest to the readers of this journal. I highly appreciate the effort of the authors to contribute to this problem, and I think that Bayesian methods are well suited to address the issue. However, I have major concerns regarding some aspects of the methodological approach of this paper. Those concerns would need to be clarified and, if necessary, corrected and the results need to be re-evaluated before I can recommend publication of this manuscript. Further-

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more, the manuscript lacks somewhat in clarity and rigor (see the specific comments).

Specific comments

Pg2Line30: Are there really “n“ linear Equations? Since k is the number of tracers, I would assume that we have a system of k linear equations. Then, if k=n we have “n” equations and “n” unknown variables. Why “n-1”?

Pg3Line14: The authors state that it is a major shortcoming of traditional mixing models that the source concentrations are assumed to come from standard statistical distributions, which are described by some parameters. The authors should acknowledge that this can be a useful approach to account for the fact that the measurements of tracer concentrations in the same source are related to each other in some way, which is a very reasonable assumption. It is a priori not entirely clear that omitting such an assumption is beneficial to solving the mixing problem, since we might neglect reasonable prior knowledge in that case. Furthermore, the authors do not directly compare the performance of their approach to the approaches they criticize (e.g. in a synthetic case study). The added value remains therefore rather vague.

Pg3Line20-25: Arguments 1) and 2) seem to be very similar, if not the same. The authors should either provide two more distinct wordings, or combine the two arguments into one. Argument 3) is not entirely clear. Of course, the true mean and variance of the entire population can only be estimated with high uncertainty from a small sample. But this can be formally considered and should not pose a fundamental problem.

Pg3Line37: Please specify what is exactly meant by the “above limitations”. The list 1)-3)? Or additional things in the text above?

Pg3Line37-46: The authors claim that the most important advantage of HydroMix is that there is no assumption about the distribution of the source tracer concentrations, if I understand correctly. While technically true, I think that this argument is misleading. Also HydroMix makes an assumption about the probabilistic nature of the model,

namely that the residuals are normally distributed with mean zero and constant variance. It is not clear to me why this should be a milder / better assumption than the one about the observations of the source concentrations being realizations of e.g. a normal distribution. All the uncertainty is just treated in a lumped way, by epsilon, which implicitly contains the deviations of the observed and the true source concentrations. Therefore, the assumptions on the source concentration distribution are not really avoided, they are just all "hidden away" in epsilon.

Pg3Line44-46: unclear what the authors mean here

Pg5Equ4: I don't understand why Eq. 4 is a solution to limitation ii).

Pg5Line11: Timestep of what? Explain what you mean by "assuming a timestep". Isn't the timestep given by the times at which the samples were taken (observed)? I don't see why "tau" can be neglected for short and long timesteps.

Pg5Equ5: what do you mean exactly by time-integrated processes? S is a state, not a process, I believe. Please clarify. You might need to provide an equation to clarify which quantity is integrated and what the lower and upper limits of integration are.

Pg5Equ6: how do "i" and "j" relate to "t"? "t" seems to disappear in the following equations. Is it reasonable to compare all the samples of the sources to all the samples of the target mixture? The authors should expand on this. When does it make sense and when not?

Pg6Line1: I believe that the citation provided here is not justified. The cited paper has nothing to do with mixing problems, it is about spectral domain likelihoods for modeling streamflow. However, it would be important to have a reference here that justifies the assumption of the Gaussian distribution for the errors in the specific case of how it is applied in this study (comparing all the measurements of source to all measurements of the mixture concentrations with normal errors). An alternative would be to check the statistical characteristics of the resulting "epsilon" and see if the normal assumption

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was justified.

Pg6Line29: Please provide the original reference for importance sampling.

Pg6Line30: Please cite original reference for the Metropolis algorithm.

Pg6Line31-33: This sentence is not entirely correct and can be omitted.

My most important comment refers to Page 6 Line 42 – Page 7 Line4. The approach that the authors chose to sample from the posterior distribution is not a valid approach. Random sampling of the parameter space with retaining the best X % of the likelihood function does not yield the correct posterior distribution. Instead, the authors obtain some arbitrary measure of spread of the parameters and neither the parameter range nor the predictions done with them have any probabilistic interpretation. This is also one of the potential reasons why they do not manage to reproduce the known “rho” in Figure 2. The true value of “rho” should be inside the confidence limits also for the overlapping (high-variance) case. Also, the higher uncertainty of the mixing ratio “rho” should be visible in the high variance case, but the estimated “rhos” seem to have the same or even less uncertainty associated to them in the high variance case than in the low variance case. This seems odd to me. I would recommend that the authors implement a proper MCMC sampler (e.g. Metropolis) to obtain an actual sample from the posterior distribution. Also, the convergence of the chains needs to be checked, either by visual assessment or by convergence tests. Only converged results should be reported, otherwise meaningful conclusions are not possible.

Pg8Eq15: Does this consider rain on snow events? This might not be so important but could be mentioned.

Pg9Line26: When are samples taken in the model? How many of them are taken? Section 4.1: From the design of the case study, it is not clear if HydroMix is a statistically coherent framework. The authors should provide a proof of concept instead of or in addition to Section 4.1. The basic design of the experiment could be similar to 4.1,

but it should be done with a large number of samples, to demonstrate that HydroMix converges to the correct solution in that case. This should also be possible for the high-variance case, I think. As I mentioned before, this should be done via proper MCMC sampling, and convergence needs to be checked. For a large number of samples, the uncertainty intervals should contain the true value of "rho", also in the high variance case.

Conclusions

As it stands, conclusion 1 is favorable and it would indicate that HydroMix is a statistically valid method, but it is not supported by the results. If one replaces the word "uncertainty" by "bias", then the conclusion is supported by the results, but it is not a favorable conclusion anymore and indicates major deficiencies of the used approach. The authors should aim to obtain results that support conclusion 1.

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