Review of: An optimal transformation method for inferring ocean tracer sources and sinks

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This paper presents a new framework to estimate oceanic tracer transport and refine measurements of air-sea flux. The framework combines ideas from water mass transformation theory and tracer transport models. The authors show several idealized, and then three more practical, applications of the framework. Currently, measurements of air-sea flux and tracer transport are uncertain, and the technique presented is a clever and promising new tool for addressing this complex and important challenge in climate science. I find the paper is well written and generally very clear for such a technical topic. I also think it's a good fit for the journal, and I expect the framework will be of interest to the community, given its broader implications for reducing uncertainty in estimates of air-sea fluxes and energy imbalance in the climate system

However, before publication, I would suggest some minor revisions. My main suggestions are that, while the paper is generally well written and clear, there are opportunities to make the method and results more physically intuitive in geographical space. Additionally, as someone who hasn't myself worked on inversion/optimization problems very deeply, I wasn't clear on the motivation behind some assumptions in the paper. Specifically, it would be useful for the authors clarify which assumptions are physically or dynamically motivated, versus those made because that's just how these problems are usually set up (i.e., because some assumptions need to be made to solve for a non-unique solution). I will give specific cases of both of these points, and more minor edits and questions, below.

Specific points:

L134: I am confused about the point regarding the EMD. The EMD method isn't being used here, right (there is no "*d*" in the equation)? I think it's the wording; what is "approach" referring to specifically? Is Q_{flux} the equivalent of the minimized cost, or of d, or of g in (3)?

L137: I'm a bit unclear on why g_{ij} acts on Q_{ij}. Is it because Q is the flux into watermass *i*, on its transit to *j*, but only the g_{ij} frcation of *i* makes it into *j*? It would help to add a sentence clarifying this here, because the previous section implies that Q is the total flux induced tracer change from *i* in *j* (i.e., as if the fraction of *i* in *j* was already accounted for).

L148: I'm confused about the motivation for this set up. If it isn't well known, why can we hope Q_{adjust} to be small? Will this force the major changes in tracer between water masses to effectively be put into g_{ij}? More broadly, is this based on a physical or practical reasoning, or is it arbitrary that you minimize Q_{adjust} and not g_{ij}? Do we assume that, in practice, the surface fluxes will be easier to guess at than the mixing? It would also help to lay out the basic idea here, or in the section on the EMD before (i.e., explain that two things are not well known, or known at all, and an established approach is to minimize the deviation in one from its prior, because the solution to (6) is non-unique). Also "non-mixing cost" isn't super clear. I would suggest explaining that or renaming.

L154) Here reiterate what solving for g_{ij} means physically… solving for the minimised mixing and advection?

Eq. 8) Here I would suggest writing instead: $\sum g_{ij} Q_{adjust} = C_{1,j} \dots - \sum g_{ij} Q_{prior}$, and then could say in the text that the total flux experienced in transit is : $\sum g_{ij}(Q_{adjust} + Q_{prior})$ or something. I suggest this because in the upcoming sections, you really only talk about Q_{adjust} adjust (not *Q*), so it is nice to have an equation to refer back to specifically. Also, to be as clear as possible for the following sections, I would suggest clarifying that the method is to use (7) to calculate g and then (8) to solve for Q_{adjust}.

L167) Related to my point above, it's not physically obvious to me why it might make sense to adjust the fluxes minimally in a per unit area sense. Could you explain? Also, it would be good to note here that you do use this assumption in some of the following examples (Eq. 15, etc).

L204) Clarify that "no cost" means the solution can be achieved with mixing alone, i.e. no adjustment to the fluxes; similar at L211.

L244) Are the dates here backwards?

Fig 3) Maybe draw the bin boundaries from Fig. 4 on these distributions (i.e., the boxes)?

L270) ...of equal volume "globally" (add globally to make subsequent statement about being different masses in each basin clear). Also, would be good to say here this is a Boussinesq model, since you are using mass and volume interchangeably.

L272) Sentence "we partition" the 16 water masses: here would be good to clarify that it becomes 16 water masses because different water masses with the same T-S properties exist in each basin.

Fig. 4: in each of the "14" bins. Also, I'm confused by the points. How are you calculating them?

Eq. 9) I had a lot of trouble with the concept of A_i here and its use in the following equations. Why is the time integral over the midpoints of the early and late periods, not the endpoints of the early period, if it's the outcrop area of watermass *i*? Instead, A_i is the average area of the outcrop of the initial watermass the time it transits to the final watermass (right)? I think that needs to be explained better since it's not immediately intuitive to me why you use this as the outcrop area over which Q acts. Also, what is the zero here in $\Omega(x, y, 0, t)$? A basin tag?

L280-281) Perhaps recall here that the following hard constraints are extensions of earlier equations (Eq. 2, etc), representing mass conservation, total tracer conservation, and transport speed/likelihood constraint.

L291) Isn't this using Eq. 15, not 7?

L295) Could you explain this a bit more (i.e., "instead of the average area over time, we skew it towards the smallest possible positive value?")

L300/Eq. 17) I'm still a bit hung up on Ω here. I think a schematic of one parcel *i*'s physical journey to *j*, in geographical space, would be helpful. This could include a diagram of the area we are using as Ω and $\mathrm{A_i}$. I think in general, this schematic would be helpful earlier in the paper to gain physical intuition of the method.

L312) Is there a reason that Q_{adjust} is constant (is it hard to get out spatial patterns)?

L335) How is up or downstream calculated? Using the streamfunction/velocity? Maybe this was explained and I missed it?

L350) I feel that this is an important point and could be highlighted more. Essentially, this technique could help provide a better estimate of the net radiative imbalance in the climate system, which is hard to do!

Fig 7) Are the dots at the boundaries of regions? Where are they coming from? Is it possible to be more continuous? Also, this is case one and two, right?

L361) "polar regions" – refer to Fig. 9 here.

Fig 8) Mention which case is shown here.

L365) Do you understand why the freshwater is more successful as a non-uniform pattern? Does the fact that the heat fluxes are minimized as a uniform pattern mean that the optimization problem might be set up imperfectly? Not the you need to do redo it, but it would help if you could mention of why this is so, if you have intuition about it.

L370) I'm not sure what "increases the cost function" means. Do you mean that it "is not a minimum of the cost function?"

L390-400) I'm curious about other dynamical ways to constrain the problem. Would it be possible to include a feature of the weights that discounts net volume transport across the strong meridional buoyancy gradients (for instance, incorporating the tendency for advection to be along-isopycnal)? This doesn't need to be discussed in the paper, I'm just curious. In the text, however, I again suggest expanding on why the assumptions regarding the prior knowledge of g and Q, were made here from a dynamical standpoint.

Fig 10) Could a panel be added with the truth? This is not required if it's really complicated... (and truth would only include the total fluxes, content change, and transport, I think). But would be nice to compare to.

L417) I would again suggest highlighting the point here that "this implies that the method, leveraged with observations, might help to refine observationally-based estimate of the net heat flux imbalance in the climate system." Or something....

Grammatical edits:
L31) Comma before "which"
L54) in space "and time"
L88) add quotations around "conservative"
L131) comma before "which"
L175) comma after "implausible"
L264) comma before "which"
L265) I would suggest replacing "volume" with "mass" since you used mass before..
L360) Remove second "of"
L361) "Adjusted" (?)