Review of Marks et al. – HESS

I want to state that I did not take part in the first round of reviews, and aside from providing my own feedback, the editor asked me to assess the authors' performance in the first round of revisions.

Presented is a conceptual study of thermobaric effects in a deep freshwater lake in the absence of wind forcing. The work introduces an expression for in situ density to account for compressibility effects at depth and uses it to examine the destabilizing effect of diffusion across $T_{MD}(p)$ as a driver of convective mixing. The authors' model appears to reproduce this type of freshwater cabbeling during winter stratification, when it would be expected. However, the absence of a mathematical parameterization limits its applicability and generalization. The paper is also hard to follow because several ideas and methods are not adequately explained or supported by analyses/figures. That said, I agree with the other reviewers and the editor that this is an interesting paper that addresses a relevant and understudied topic in deep, freshwater systems.

I do not see significant improvements over the initial version. The authors missed the chance to address much of the feedback they received, as reflected in the few changes made to the manuscript. Furthermore, I have rarely seen a paper returned with major revisions that does not modify any graphical displays (one reviewer explicitly asked for a schematic or at least a modification to one of the figures, which was not done). The authors' approach in the Open Discussion and revision seemed quite dismissive, particularly regarding comments about the choice of equation of state. Many responses were limited to underdeveloped arguments. Including calculations and figures to support those arguments would have strengthened the discussion. Overall, I would have liked to see more scientific engagement from the authors.

Below, I provide feedback and comments that may seem extensive for a paper in its second revision round. My goal is for the authors to engage with the proposed discussion and ultimately include some relevant points in a new section addressing the limitations of the study. I also strongly urge the authors to include a schematic drawing of the studied process, illustrating what occurs in the water column and highlighting how the model's different modules contribute to representing it. This will help the community in following your ideas.

Comments on TEOS-10 discussion

The gray text in this section details comments or viewpoints that I could not refrain from stating. But I would only expect a response and modifications concerning the part in black.

The authors are correct in noting that TEOS-10 is an instrument developed to deal with the properties of seawater. But I would like to stress that the work by Pawlowicz and Feistel's (2012) is highly relevant because it provides a method to extend the thermodynamically conservative framework of TEOS-10 to freshwater systems when accounting for lake-specific ion content. Expanding the study of freshwater thermobaric effects in environments with salinity gradients would be challenging without such a framework, and I believe there's a reasonable trade-off between possible loss of accuracy/precision and the advantages of a robust framework that enables consistent calculation of all relevant thermodynamic quantities.

The TEOS-10 thermodynamic equations have been validated for pure water, and the temperature ranges for cold pure water discussed in this manuscript are well within the 'oceanographic funnel' defined by

McDougall et al. (2003 JAOT) and implemented in the TEOS-10 package. It may well be that Tanaka et al. (2001)'s density formulation for pure water is more accurate, but the differences from TEOS-10 are minor (see figure below), and I remain unsure whether that greater accuracy offers a real benefit for the manuscript's purpose (see following paragraph).

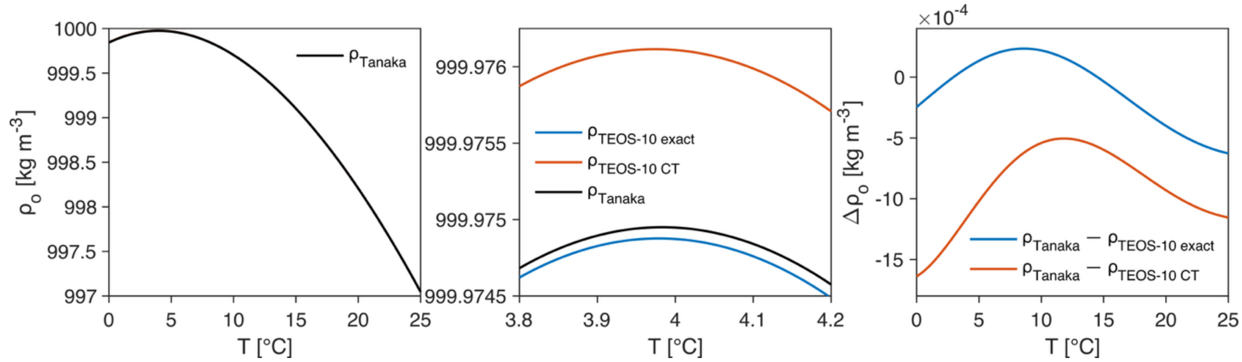

Figure 1: Comparison of Tanaka's with TEOS-10 densities at atmospheric pressure. The $\rho_{TEOS\text{-}10\ CT}$ corresponds to the density calculated from conservative temperature (CT) and absolute salinity (SA; in this case, SA=0) using the computationally efficient expression (75-term equation) for specific volume in terms of SA, CT and pressure (Roquet et al., 2015 OM). For this calculation, CT was obtained from in situ temperature and SA=0 at p=0, but the result is plotted as a function of the original (in situ) temperature.

Anyhow, the constructive criticism raised by the reviewers, in my opinion, has nothing to do with the accuracy of the density value at atmospheric pressure, but rather with the use of conservative temperatures for pure water, as defined in TEOS-10, which provides a thermodynamically conservative framework that could benefit the study. McDougall and Barker (2014 JGR: Oceans) argue that operating on a quantity like in situ density, which is neither potential nor conservative, causes unwanted nonconservative production or "artificial" mixing, with cabbeling being a known example (potential temperature will also pose problems). At the narrow range of temperature fluctuations in which thermobaricity may play a role in freshwaters, this artificial mixing could be significant. I understand that Piccolroaz & Toffolon (2013 JGR) correct for artificial mixing after their stabilization algorithm. In the present manuscript, the authors have not considered this type of correction. Since both their diffusion and stabilization (or mixing?) algorithms rely heavily on averaging, I am concerned that the cabbeling they report, although a plausible process, may be significantly amplified by their choice of equation of state. I strongly recommend discussing this potential limitation in the manuscript.

The buoyancy frequency described in the paper is nearly equivalent to the widely used "adiabatic leveling method" (see e.g., McDougall and Barker, 2014 JGR: Oceans, eq. 10 therein). This method, attributed to Millard et al. (1990 DSR), is the reference cited by Peeters et al. (1996) when defining buoyancy frequency, so I think it deserves mention. But most importantly, it is because eq. 10 in McDougall and Barker (2014) is equivalent to their eq. 1f using potential densities at the same locally referenced pressure, that the leveling method is adequate to calculate buoyancy frequency. Also note that strictly speaking, the furthest right-hand side of the present manuscript's eq. 6 is not directly equal to the rest of the equation. Using, e.g., i and i+1 indices instead would be preferable to avoid abuse of notation.

Proposed expression for in situ density

Working with in situ density is undesirable as this quantity is neither potential nor conservative. That said, my main problem is that I do not follow the way the authors calculate the integral in eq. 3. The provided information does not allow the reader to assess the deviation of the Taylor expansion around p=0 (eqs. 4 and 5) for depths far away from the surface. Since you have an expression for the speed of sound as a function of potential temperature and pressure, why don't you integrate eq. 3 numerically? Did you verify your derived expression against such an integral? If I plot the in situ density of pure water for a potential temperature profile similar to your winter stratification data at great depths, I only see an increase in density with pressure (as in the Fig. 2 inset of Peeters et al., 1996). For 2 m bins in your model, I struggle to imagine any temperature fluctuation that would overcome such pressure dependency when analyzing the stability of the water column using the resulting in situ density. There are validated polynomial expressions for in situ density that can be used for pure water, assuming S = 0 (S_A = 0), such as Chen and Millero (1986 L&O) (or TEOS-10). How does your in situ density expression (eq. 5) compare to that of Chen and Millero (1986; eq. 1 therein) at different pressures? Please provide a graph in your response.

Following this comment, it would be of tremendous help for the reader if, in the paper, you show plots of in situ (and potential) density before and after the "stabilization" algorithm. Particularly at depths around T_{MD} when diffusion would be expected to generate cabbeling during the winter stratification. A waterfall plot showing several sequential profiles of in situ (and potential) density and potential temperature, before (e.g., dashed line) and after (continuous line) stabilization, with a constant time-dependent offset, could be informative for understanding what the model does.

Numerical model

I really struggle to follow the modeling procedures because the manuscript provides no mathematical description of the model. It is nice that you shared your code, but that does not mean the reader needs to go through your code to follow your work. I understand that diffusion and convection are modeled sequentially, with the latter implemented via the stability algorithm (a schematic of the algorithm would be really helpful to the reader). However, the lack of a description of the numerical implementation made me wonder about diffusion modeling and boundary conditions (I'm guessing you intend Dirichlet at the surface and no-flux Neumann at the bottom boundary?). Upon reviewing the code, I noticed that the diffusion algorithm implemented is a form of curve smoothing through averaging rather than a straightforward numerical solution of the diffusion equation. In my opinion, this approach lacks justification because (i) implementing a time-implicit solution of the diffusion equation is not difficult, and (ii) the prescribed diffusivity coefficient may significantly affect the development of an unstable profile due to diffusive transport across the T_{MD} as a function of depth. If diffusion is, for example, unreasonably amplified at every time step, there is no way to discern whether the model generates artificial mixing through diffusion-induced cabbeling. Also, regarding (i), I am surprised this was not noted in the first round of revisions, and I firmly believe that validation against a numerical solution or benchmarking against a known theoretical 1D diffusion problem with a theoretical solution is largely missing. Previous 1D vertical minimal models, such as those from the group at the University of Trento, solve the diffusion equation numerically using a time-implicit method, and the authors should have built on those models for their work (the group at the University of Trento has many codes available publicly online).

I acknowledge that the approach seems to work even without explicitly modeling diffusion as I would expect. However, I am uncertain whether cabbeling is adequately incorporated with the chosen approach. Providing more details, such as figures, showing what the model does at each timestep would be helpful. That said, the work could greatly benefit from implementing diffusion using a time-implicit method. This approach would also establish a mathematical framework for properly applying boundary conditions. Additionally, by testing how sensitive the simulation is to different prescribed background vertical diffusion coefficients, the authors could better assess the role of cabbeling instability in the generation of convective mixing.

Reviewer 1 asked about the effect of changing the diffusion coefficient. I find the author's response deficient because they argue about something their current model is unable to assess, as it cannot prescribe the diffusivity coefficient. In the same response, the authors argue that "In general, the strength of the diffusion does not change the behavior of the deep mixing at all, it only defines the vertical scale of the mixed surface layer by controlling how much cold/warm water during winter/summer is transported downwards." If this were true, then it would imply that the stability model dominates the generation of mixing. But, in the context of studying thermobaric effects, isn't the goal of a stabilization procedure to resort the water column following the adiabatic path and leave mixing to turbulent diffusion? Going back to the artificial mixing mentioned earlier, this statement raises more concerns than certainties.

Regarding the model's diffusivity reported in the manuscript ($5.5{\times}10^{-4}$ m^2 s^{-1}), I guess this is an effective value calculated a posteriori, right? But could the authors mention how they obtain this value in their methods? Is this obtained using something like the flux gradient method from Powell and Jassby (1974 WRR) for the model output? I do not see why the authors cite an article by Saber et al. (2018), which has nothing to do with thermobaric convection, to support the reported value. Also note that a diffusivity value of $5.5{\times}10^{-4}$ m^2 s^{-1}, although not excessively large, is still larger than the average oceanic diffusivity ($\mathcal{O}(10^{-5})$ m^2 s^{-1}; Waterhouse et al. 2014 JPO), so I would suggest discussing a bit more the reported value. What would be the resulting effective diffusivity if only the diffusion or stabilization module were to be active in the simulation?

Finally, regarding the stabilization model, I would appreciate a discussion on why the authors consider it appropriate to prescribe the surface layer temperature for a large portion of the water column during stabilization. I can see how instabilities are removed, but wouldn't this alter the water column's potential energy in an undesirable way?

Minor comments

1 Clarify potential misinterpretation in the title. The current version is an improvement, but the reader may still think that the paper covers wind-induced thermobaric instability. I'd suggest being explicit about the absence of wind forcing.

2 In Fig. 1, because of the color choice (bright blue versus pale tones) and display order, the lake's bathymetry stands out. While you argue that the lake's bathymetry justifies the 1D approach, I believe the most relevant part of the figure is the profiles measured in April 2005, which show T_{MD} crossing and a deep, nearly isothermal characteristic. Also, the map looks pixelated and sloppy.

3 What is the point of Figure 2? If the goal is to show the stratification inversion, then it could be more targeted to the first 100 m. If you want to show what's happening across the whole water column, perhaps contour plots of $T - T_{MD}$ would be more appealing (the $T - T_{MD} = 0$ crossing during winter stratification should depict where cabbeling is expected – if pursued, a diverging colormap, pivoted at 0, would also be recommended).

4 Line 98: "Potential density $\rho_{pot} = \rho_{pot}$ (T) is a function of (potential) temperature at a certain reference pressure". While I understand what the authors mean, I do not fully agree with this statement. I prefer the TEOS-10 definition "Potential density is the density that a fluid parcel would have if its pressure were changed to a fixed reference pressure in an isentropic and isohaline manner". The way these

concepts are presented in the paper is somewhat misleading, since, theoretically, potential density is defined as an integral function of in situ density and compressibility. In the manuscript, it appears as if potential density comes first— I am guessing for practical reasons. Yet the wording of that section could be improved.

5 An isothermal initial condition of 4.2 °C for potential temperature in the model would imply that the surface and bottom in situ temperatures differ slightly. Is this the intended setup? I'd really like to see in the paper the Salinity of profiles shown in Fig. 1b (or was conductivity below the detection limit?). While I fully understood that the paper does not deal with salts, it would help to clarify the isothermal characteristic shown in Fig. 1b, which is then used as the initial condition for the model. Also, the data shown in Fig. 1b is expressed as potential temperature, right? Since the use of potential temperature is clarified later in the manuscript, I suggest noting the use of potential (or in situ) temperature in the labels and caption of Fig. 1b. Using more common notation like θ and ρ^{θ} for potential temperature and potential density, respectively, would help avoid confusion (e.g., Peeters et al. 1996)

6 There are two recent papers by Eddy Carmack on thermobaric effects in cold, deep lakes that I think are worth mentioning.

- Carmack, E., & Vagle, S. (2021). Thermobaric processes both drive and constrain seasonal ventilation in deep Great Slave Lake, Canada. Journal of Geophysical Research: Earth Surface, 126, e2021JF006288. https://doi.org/10.1029/2021JF006288
- Carmack, E., Vagle, S., & Kheyrollah Pour, H. (2024). Seasonal temperature and circulation patterns in a hybrid Polar Lake, Great Bear Lake, Canada. Journal of Geophysical Research: Earth Surface, 129, e2024JF007650. https://doi.org/10.1029/2024JF007650