Review of: The interpretation of temperature and salinity variables in numerical ocean model output, and the calculation of heat fluxes and heat content By McDougall, Barker, Holmes, Pawlowicz, Griffies, and Durack

Summary and recommendation

This main goal of this paper is to develop arguments seemingly making it possible for the potential temperature (PT) of EOS80-based models to be `interpretable' in some sense as Conservative Temperature (CT), which if true, would allow ocean modellers to directly compare the PT of EOS80 ocean models with the CT of TEOS10 ocean models, instead of comparing the like for like, which has been the accepted practice so far.

This paper is difficult to review and understand because it relies nearly exclusively on nonstandard arguments and abstract reasoning, as well as on nonconventional views about the nature of ocean models and of their dependent variables. In my first review, my initial reaction was that the paper had to be wrong, but I was not able to fully pinpoint exactly why. Having now read the paper 3 times and having had more time to reflect on its message, I now understand that the primary cause of my discomfort is the fact that this paper appears to assume that the evolution equation and boundary conditions satisfied by a physical quantity have some bearing on the definition of such a physical quantity, which seems to conflict with what is normally assumed in standard physics (at least, the way I understand it).

Take potential temperature for instance. As is well known, such a physical quantity is generally regarded as being rigidly defined as the notional temperature that a parcel would reach if brought adiabatically to the ocean surface at the mean atmospheric pressure, which is sufficient to fully define it. In particular, the evolution equation and boundary conditions that we may then formulate to predict its temporal definition are not normally supposed to have any bearing on its definition. Indeed, according to my understanding of physics, the definition of a physical quantity and its assumed evolution equation are generally regarded as entirely separate businesses. It follows that if we decide to approximate the evolution equation and boundary conditions for PT instead of using the most accurate one available, the usual view is that this will only introduce errors and uncertainties in the simulated PT, but not alter the character of PT itself. In this paper, however, the authors appear to take a different view. Specifically, they contend that if the evolution equation used to predict the temporal behaviour of PT is not the most accurate one available, but an approximated version of it that resembles the evolution equation for CT, then PT loses its PT character somehow to assume that of CT. Thus, even if PT is initialised with observed values of PT and if the equation of state used assumes PT as its argument, the authors contend that PT will drift towards CT after some `long spin-up time' if PT is treated as strictly conservative. (The authors do not provide the evolution equation supposed to be satisfied by the drift, nor do they discuss the physical quantities controlling the relaxation time scales controlling the drift, which would allow us to check the authors' views).

Having realised that the main cause of my discomfort was due to the authors allowing the evolution equation and boundary conditions satisfied by a physical quantity to interfere

with its definition, in contrast to what I think is the normal practice, it became much easier to understand the reasons for otherwise many very unclear statements and assertions. For instance, it now made more sense to me why Prof. McDougall and the authors would contend that potential enthalpy should be regarded as the variable defining heat content in the ocean. Indeed, a review of the literature on the subject (Bryan 1962; Bacon and Fofonoff 1996; Saunders 1995; Warren 1999) prior to McDougall (2003) clearly reveals that the quantity $c_{n0}\theta$ used so far as definition of heat content had been regarded as some approximation to the non-mechanical part of the total energy, its 'heat' quality resulting from the difficulty to convert it into mechanical energy, as per the second law of thermodynamics. Indeed, what standard thermodynamics tells us is that the 'heat' forms of energy cannot be converted with 100% efficiency into `work' forms of energy. In the classical view, therefore, 'heat' is regarded as a property of the fluid, as a form of energy that is difficult to convert into mechanical energy, irrespective of how surface heat transfer affects it. The authors appear to take a completely opposite view, however, namely that potential enthalpy is the relevant definition of heat because its surface flux captures the entirety of the surface heat transfer, irrespective of its degree of convertibility with mechanical energy. This is why in my first review I expressed the opinion that Prof. McDougall's approach was idiosyncratic, not to cause offence, but to point out how radically different its premise appeared to be compared to that of previous approaches. My criticism was addressed to the fact that the authors appeared to present their arguments in support of potential enthalpy as the relevant definition of heat as being self-evident, without mentioning to the reader how different its premise is compared to that of previous approaches, nor its ad-hoc character. For instance, adopting the authors' views, how would one define heat if the ocean were in fact primarily thermally forced along its uneven topography? As potential enthalpy referenced to a spatially varying bottom pressure? But then, heat would be a function of potential temperature, salinity, and horizontal position. Would that be acceptable? From a more fundamental viewpoint, shouldn't one seek a definition of heat that is equally applicable to the atmosphere as to the ocean?

To go full circle, the authors also contend that the salinity variables used in models should be interpreted as preformed salinity, on the grounds that current ocean models treat such variables as strictly conservative, which the authors argue is true only of preformed salinity. According to the authors, both temperature and salinity variables will 'drift' towards CT and S* after some undefined 'long spin-up time' regardless of how they are initially defined or initialised provide that they are treated as strictly conservative.

Because my understanding of physics is that the assumed evolution equation and boundary conditions of a physical quantity have no bearing on the definition of a physical quantity, my view is that the paper is based on unsound physics. Now, I also must acknowledge the fact that this paper touches on fundamental aspects of physics that are rarely if ever explicitly discussed. The fact that such eminent oceanographers appear to have such a different understanding of physics than I, combined with the fact that the views expressed in this paper did not appear to bother the second reviewer, Prof. Fox-Kemper, a lead author of a chapter in the latest IPCC report, suggests that the issues touched upon are not well understood by the community, and hence that there may be value in publishing this paper along my review in order for the community to reflect on where it stands on the issues discussed.

Major issues

Potential source of divisions – In the event that only part of the ocean modelling community adopts the authors' recommendations, with the remaining part disagreeing with them and therefore sticking to the currently accepted practices, what would be the authors' suggestion for resolving the resulting schism in the community? Wouldn't it be wise/useful for the SCW or the CLIVAR ocean modelling working group to organise some kind of worldwide poll about the issues discussed to identify to what extent oceanographers agree or disagree with the authors' view that it is ok for the evolution equation and boundary conditions to interfere with the definition of a physical quantity? I hope that the authors can agree that the development of incompatible ocean modelling practices cannot really be good for the field and is likely to complicate the writing up of the 'ocean' chapter of the next IPCC report. It seems to me that the authors should address this issue in their paper, i.e., the possibility that not everyone will agree with their recommendations.

Specific comments

Line 68 – Saying that density depends on 'heat content' is dangerous and provocative since the concept of 'heat content' is controversial and likely to remain so for the foreseeable future. Why not stick to uncontroversial and non-provocative practices?

Lines 70-71 – I don't understand the point here. The evolution equations for potential temperature and conservative temperature are non-conservative, whether we think it is useful or not. Treating such quantities as conservative necessarily entails an approximation that is the modellers' decision and has nothing to do with the conservativeness of the numerical schemes.

Lines 73-74 – Some numerical ocean models formulate their temperature equation in advective form, in which case the said conservative property is not satisfied (as far as I am aware)

Lines 77-79 – It is precisely for the same reasons that many scientists advocate that one should close the energy budget of ocean models, which cannot be done without retaining the non-conservation of heat in the temperature equation of ocean models, e.g., Tailleux (2010), Dewar, Shoonover, McDougall and Klein, Fluids (2016).

https://doi.org/10.3390/fluids1020009

The authors make the implicit assumption that models that treat their temperature variable as conservative but not their total energy are more reliable than the models doing the opposite, i.e., treat their total energy as conservative but not their temperature variable. Shouldn't this be left as an open issue for the community to think about?

Line 97 – I don't understand the term `contradictions' being used here. Anybody else would describe the approximations made as resulting in errors/uncertainties in need of being quantified, not contradictions. The terms neglected have been shown to be small, and therefore consistently neglected by ocean modellers. Even if one agreed to use the term

'contradiction' here, logic would dictate that resolving the contradiction would be to use the correct equation for potential temperature. Arguing that one should switch to conservative temperature may be a viable alternative, but it is not the logical choice that follows from saying that neglecting some terms in the potential temperature is illogical or contradictory, since the contradiction is eliminated by retaining the terms that the authors say one should not neglect.

Line 99 – May be the 'contradictions' that the authors refer to have been ignored because they are not real contradictions, and just simply because the terms neglected are so small that retaining them would not make any difference, which would be the natural thing to discuss.

Lines 103-104 – 'at the cost of introducing problems elsewhere'. This seems a very strange line of reasoning to me, as the analysis of the problem clearly reveals that the problem that the authors discuss can easily be corrected without introducing any problems elsewhere, by using the correct equation for potential temperature instead of the approximate one. I find it hard to understand why the authors find it worthwhile to discuss inferior solutions.

Lines 109-111 – "For example, the insistence that a model's temperature variable is potential temperature involves errors in the air-sea heat flux in some areas that are as large as the mean rate of current global warming" – This is just not true, because the problem that the authors raise is not due to using potential temperature as such, but with not using the exact evolution equation and boundary conditions for it. As shown by Tailleux (2015), correcting the equation for potential temperature to address the authors' criticism would be very easy to implement. It is misleading for the authors to put the blame on potential temperature, where the blame lies in fact with ocean modellers not using it most accurate equation for potential temperature is a great temperature variable, which has the properties that it has, and there is a priori no problem in using it if the correct evolution equations and boundary conditions are used. IOC et al. (2010) clearly misunderstands this. The best practice is not using CT instead of PT. The best practice is to use the most accurate evolution equations and boundary conditions, regardless of which variable is used, both variables being perfectly acceptable if used consistently.

Line 165 – 'has a mean non-conservation error' Why do the authors call it an 'error'? The non-conservation of any temperature variable is a real physical process as far as I am aware.

Line 165 – The authors need to say that the number of '0.3 mW m-2' relies on neglecting the non-conservation of potential enthalpy arising from the Joule heating due to the viscous dissipation rate, and that if the latter was retained, this number would be much larger and not that different from that for potential temperature.

Line 178 – As pointed out in my first review, the viscous dissipation must balance the mechanical power input by winds and tides, which provides a useful sanity check. 3 TW is a very lower bound for this, which amounts to 10 mW/m2, which is more than 3 times larger than that of Graham and McDougall, 2013. Graham and McDougall 2013 estimate is therefore implausibly too small.

Line 181 – Potential enthalpy had been in used as the thermodynamic variable used in the GISS model, as pointed out in my first review. It would seem justified to cite Russell et al. here, and point out that the variable has been in use way before McDougall (2003) re-discovered it.

Line 195 – Why is potential temperature not conservative?

This paragraph seems to mix up the a priori unrelated issues of 'conservativeness' and 'how to define heat content'. For clarity, it would be best to discuss the problem of how to define heat somewhere else, since the two issues are only indirectly related. I also find it strange that the section title only mentions potential temperature, given that the physical reasons why `heat'-like variables are non-conservative are a priori the same for PT and CT, so why leave CT out of the section title?

As to the explanation for non-conservativeness, the simplest in my view is to say that both PT and CT are non-conservative because:

- Neither PT nor CT mixes linearly (under diffusive effects alone), i.e., the PT or CT of the mixture of two water samples is different from the mass weighted average of the two samples.
- In a turbulent ocean, PT and CT also systematically increases during mixing events due to turbulent dissipation of kinetic energy by viscous processes

Then, the conditions can be separated for PT and CT. For instance, the authors could say that the non-conservativeness of CT is controlled by the temperature dependence of T/θ whereas the non-conservativeness of PT is controlled by the temperature dependence of $T c_{pr}/\theta$ – If c_{pr} were assumed constant and T/θ were a function of pressure only, as for a dry atmosphere, then both CT and PT would be considerably more conservative than in seawater and would have identical degree of non-conservativeness. The fact that PT is less conservative than CT is due to the temperature dependence of c_{pr} – with a lesser role for the salinity dependence. This is shown by Eqs (23) and (25) of Tailleux (2010), which I think the authors should refer to. The method developed by Tailleux (2010) (or Tailleux (2015)) is the most general currently available and is valid for the full Navier-Stokes equations. At the moment, this method is the one that underlies the construction of energetically consistent approximations. The methods discussed in IOC et al. (2010) and Graham and McDougall (2013) are much less general. Moreover, they fail to incorporate viscous dissipation as part of the definition of non-conservation of PT and CT.

Line 215 – "This suggestion has been made, for example, by Tailleux (2015)" First, I don't think that the suggestion has been made by anybody else. Second, the method proposed by Tailleux (2015) is merely to make use of the passage relations $\theta = \theta(S_A, \Theta)$ and $\Theta = \Theta(S_A, \theta)$ to reformulate the evolution equation for CT used by a TEOS10 to obtain a mathematically equivalent one but for potential temperature. In other words, the evolution equation for potential temperature can be obtained by a simple change of variables from that for conservative temperature. Alternative, one could also diagnose the nonconservative terms in the evolution equation for potential temperature to close the energy budget of the EOS80 numerical ocean model considered, as in Tailleux (2010). Both strategies circumvent the difficulties raised by the authors and show that improving the equation for potential temperature would be a trivial exercise. Given that both Tailleux (2010,2015) have proposed concrete solutions to compute the nonconservative terms to be added to the evolution equation for potential temperature, I find it odd and rather non-collegial for the authors to assert that such approaches would be unworkable. If the authors do not understand how to improve the evolution equation for potential temperature, this does not mean that is necessarily true of everybody else. Instead of unfairly disparaging Tailleux's work, the authors could simply say that Tailleux's suggestions remain to be implemented and tested and compared with a CT-based formulation.

Lines 239-242 – I think that the authors misunderstand and misrepresent Tailleux (2010,2015)'s approach. Indeed, Tailleux (2010)'s approach is fully deductive and rigorous, contrary to what the authors seem to suggest. Specifically, Tailleux's approach to obtain a mathematically explicit expression for the non-conservation of CT an PT is identical to that used by Prigogine and the Belgian school of non-equilibrium thermodynamics (improved by Lesley Woods, 1975) to obtain a mathematical expression for the non-conservative production of entropy. Physically, this approach consists in defining the non-conservation of specific entropy (and by extension that of CT or PT) as what is needed to make total energy conservative as per the law of energy conservation. Here, the term 'conservative' means that all the terms entering the evolution equation for total energy can be written as the divergence of a flux, which is the usual definition. In their paper, the authors seem to confuse the term 'conservative' with the property of 'mixing linearly', as when they say total energy is not conservative they clearly mean that total energy does not mix linearly. Saying that total energy is non-conservative is very confusing.

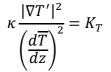
Now, the full evolution equation for the specific enthalpy in seawater takes the form:

$$\frac{Dh}{Dt} = -\frac{1}{\rho} \nabla \cdot \left(\rho F_q\right) + v \frac{Dp}{Dt} + \varepsilon_k$$

(see Eq. B19 of the latest version of TEOS10 manual with remineralisation term removed) In a turbulent ocean, neither the pressure term nor turbulent viscous dissipation can be neglected, so Graham and McDougall (2003) assertion that the locally referenced potential enthalpy mixes linearly if one neglects viscous dissipation is inconsistent with the fact that pressure always fluctuates in a turbulent ocean. However, it appears to be true that the first-principles expressions for the non-conservation of CT and PT obtained by Tailleux (2010) can also be obtained by treating specific enthalpy as if it were linearly mixed, i.e., by omitting the pressure term in the above equation. However, because Tailleux (2010) and Tailleux (2015) are rooted in a fully deductive and first-principles approach, which is not the case of Graham and McDougall (2013), the correct way to justify the assumption made by Graham and McDougall (2013) is by showing that it follows from the exact results of Tailleux (2010), not the reverse.

Lines 253-256 – 'However, these expressions are written in terms of molecular fluxes and it is not possible to use these expressions to evaluate the non-conservation in a turbulently mixed ocean' I really don't understand where does this come from. Again, the authors appear to assume that because they do not know how to do something, this should also be the case of everybody else, which seems to me to go against the collegial nature of science.

Moreover, the Navier-Stokes equations are well accepted to describe both laminar and turbulent motions, so clearly Tailleux (2010,2015)'s expressions pertain to a turbulently mixed ocean, contrary to what the authors say. What is true, however, is that the expressions remain to be linked to turbulent fluxes or microstructure measurements in order to allow for their evaluation. One way this could be done is by using expressions such as the Osborn-Cox model linking the dissipation of temperature variance to the turbulent heat diffusivity as follows:



In the left-hand side, the terms involve the molecular fluxes of temperature as well as the mean temperature profile, whereas in the right-hand side appears the turbulent diffusivity for the mean temperature. The authors' remarks have incited me to rework on the issue in order to show that such expressions can indeed be linked to microstructure measurements and evaluated from first principles, as I hope to show in a forthcoming publication.

Line 331 – What this describes is 'density salinity' – My understanding is that density salinity is always different from absolute salinity except when all the haline contraction coefficients for each of the chemical constituents are identical. May be this can be mentioned and commented upon.

Line 341 – Can the authors clarify whether the relation is actually between S* and SA, or between S* and SD (density salinity).

Lines 361-367 – Can the authors comment on the differences in computational efficiency of the equation of state between the Jackett and McDougall (1995) and Roquet et al. (2015). This information is important for ocean modellers to decide whether to switch or not to switch.

Lines 381-392. I agree that TEOS10 has conclusively shown that variations in composition potentially matters for estimations of the thermal wind. However, it is also essential that the equations of motion used by ocean models be mathematically and physically well posed. As far as I understand the problem, while it is obvious that the equations of motions based on the use of reference composition salinity are well posed, it seems to me that this is not the case if we use absolute salinity (or rather density salinity). Moreover, as well as making the equations of motion ill posed, the use of density salinity also seems to screw up the energetics by introducing spurious sinks and sources of energy. As far as I am aware, TEOS10 never wrote down a mathematically consistent set of equations about the importance of the variations in composition accompanied by the authors writing down a full set of equations of motion that can be studied by mathematicians and dynamicists like me. If the authors cannot produce a mathematically well posed set of equations using absolute salinity, it seems to me that they should not promote it as a meaningful basis for ocean modelling. If model equations using absolute are ill posed as I think they are, the

consequences is that it is a priori impossible to be sure of how to interpret the results of McCarthy et al. (2015). To me, this is a key issue that the IOC et al. (2010) and the authors appear to have overlooked.

Line 406 – What is the way to compute Cp(S*,theta,0) using the TEOS10 software? Can they provide the appropriate lines of code that would need to be invoked to compute it?

Line 412 – The fact that the authors use sometimes S^{*}, sometimes SA is confusing.

Lines 414-415 – May be add a physical explanation for why the temperature or rain is not treated consistently.

Lines 444-445 – That's the authors interpretation. The alternative and more common interpretation is that these errors are accounted for in the estimation of errors and uncertainties affecting the simulated PT field.

Lines 453 – To ensure that the model equations are well posed, many ocean models will assume that salinity argument is reference salinity rather absolute salinity. Again, I have yet to see a consistent set of equations based on absolute salinity.

Lines 481-488 – I think that this paragraph is going to cause considerable confusion in the community as it seems inconsistent with the way things have been described before. First, IOC et al. (2010) says that the new equation of state is defined in terms of absolute salinity (while in fact using density salinity to estimate absolute salinity, even though the two are supposed to be somewhat different). Now, the authors appear to say that it is defined in terms of preformed salinity S*, which is always numerically different from absolute salinity. Does that mean that the authors are actually already moving away from the recommendations of TEOS10? Nothing of what the authors say about salinity in this paper makes any sense to me. I just don't understand where all this come from, and I suspect I won't be the only one. I think that it would greatly help if the authors could write the model equations that ocean modellers are supposed to solve with the proposed interpretation, may be in an appendix.

Lines 489-492 – What is this based on exactly?

Lines 499-503 – "The model's salinity variable will drift towards being preformed salinity." I really don't understand why. How can the authors make such an assertion without substantiating it. For instance, could the authors write down an evolution equation for the drift that would clarify the relaxation time scale and convince us that what the authors describe has a counterpart in the mathematical world?

Lines 536 – This is not how models work. Indeed, as far as I understand the issue, the temperature variable used by a model is not a matter of interpretation, it is a matter of declaration. The first step in constructing a model is to declare what its dependent variables should be. Once the variables have been declared, the next step is to decide on the evolution equations and boundary conditions that one will use to describe their temporal evolutions. To me, it is essential that models be based on precise definitions and

declarations, not interpretations, so that what we do can be easily understood by our colleagues mathematicians and atmospheric scientists. I am pretty sure that mathematicians cannot understand what the authors mean by 'interpretation', which is bound to leave them very confused. My impression is that the authors use the term 'interpretation' because they want the reader to accept their view that the physical meaning of the variables used by an ocean model is open to discussion, which seems questionable at best.

Line 543 – I disagree that this is a conclusion. It looks much more like an opinion or assertion. It would be useful if the authors could provide the reader with some experiments to run that would enable the ocean modelling community to test its validity.

Lines 556-557 – Again, my view is that the evolution equation and boundary conditions have no bearing on the definition of a physical quantity. For this statement to be acceptable, one has to accept that the definition of a physical quantity is not independent of its assumed evolution equation and boundary conditions, in contrast to what is generally done (as far as I understand it).