Thermodynamics/dynamics coupling and thermodynamic consistency of Boussinesq and anelastic binary fluids with an arbitrary nonlinear equation of state

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This paper shows that the energetics of Boussinesq and anelastic fluids possesses a term that can be identified as the approximation $\delta W_{ba}$ to the compressible work of expansion/contraction $\delta W = -P \delta v$, where $P$ is the pressure and $v$ is the specific volume. It follows that Boussinesq and anelastic fluids admit explicit compressible effects and conversions between internal energy and mechanical energy, under the form of apparent changes in gravitational potential energy resulting from changes in density by diabatic and adiabatic effects. From the knowledge of $\delta W_{ba}$, the corresponding approximation to the "heat" $\delta Q_{ba}$ can be constructed in a consistent way by requiring that the Maxwell relationships be satisfied, ultimately leading to the construction of a well defined approximation to the internal energy and ultimately of the full range of known thermodynamic potentials. These properties make it possible to endow common forms of the Boussinesq and anelastic approximations with fully consistent energetics and thermodynamics, even when diabatic effects and an arbitrary nonlinear equation of state for a binary fluid are retained, without loss of accuracy. In that case, it can be shown that the sum of kinetic energy and enthalpy is a conservative quantity, which plays the role of the total energy in the Boussinesq and anelastic approximations for both diabatic and adiabatic motions. This implies that gravitational potential energy can be regarded as the difference between enthalpy and internal energy, and hence as a pure thermodynamic property of the fluid.

An important implication of the present results is to support the recent suggestion by Tailleux (2009) that the Boussinesq approximation is capable of describing potentially large conversions between internal energy and gravitational potential energy in turbulent stratified fluids, which physically seems to require that an active role be played by the emission and dissipation of acoustic waves by molecular diffusive heating and cooling, as well as by the associated divergent velocity field, a surprising result with potentially important implications for our understanding of turbulent mixing in stratified fluids if further confirmed. Another implication of the results is to suggest that the form of the Boussinesq primitive equations currently used as the basis for a majority of numerical ocean models possesses a potentially significant spurious source of momentum, which can in principle be corrected by using an alternative and more physically-based definition of buoyancy in the hydrostatic approximation.
1. Introduction

Many fluid flows of interest in engineering and geophysical fluid dynamics have low Mach number ($M = U_0/c_s$) and small relative density variations ($\rho - \rho_0/\rho_0$, where $U_0$ is a typical velocity scale, $c_s$ is the speed of sound, $\rho$ is the density and $\rho_0$ a reference density. It has been common practice over the past century to regard such flows as incompressible or weakly compressible, where an incompressible fluid is one whose density dependence upon pressure is eliminated while still possibly retaining its dependence upon temperature (and chemical composition as the case may be), e.g., Lilly (1996). There has been much effort in seeking to take advantage of the smallness of the two above parameters to develop sound-proof reduced sets of equations that are somehow simpler to study than the fully compressible Navier-Stokes equations. Two particular classes of approximations have been particularly influential and key to simplifying the numerical and theoretical analysis of low Mach number fluid flows, and will be under focus in this paper. The first one is the Oberbeck-Boussinesq approximation (after Oberbeck (1879) and Boussinesq (1903)), which in its most common form retains only the rotational divergence free component of the velocity field, and treats the density as constant everywhere except where it multiplies the acceleration of gravity. The second one is the Anelastic approximation, e.g., Ogura & Phillips (1962); Lipps & Hemler (1982); Bannon (1996); Durran (1989); Ingersoll & Pollard (1982); Ingersoll (2005); Pauluis (2008). Many other sets can be constructed, which are beyond the scope of this paper, for instance by using low Mach number asymptotics and multi-scale expansion techniques, e.g., Müller (1998); Klein (2009, 2010). Davies & et al. (2003) offers a review of a number of commonly employed reduced sound-proof sets of equations, and show how they respectively represent normal modes on the sphere.

The main focus of this paper is on how compressible effects and the coupling between mechanical energy and internal energy (the dynamics/thermodynamics coupling) are represented in the Boussinesq/anelastic approximations, which are known to decouple either fully or almost fully the thermodynamics from the dynamics for adiabatic motions and a linearised equations of state, i.e., Spiegel & Veronis (1960); Ogura & Phillips (1962). In the latter case, the Boussinesq/anelastic approximations usually admit a well-defined conservative energy quantity, e.g., Lilly (1996), but the issue of the energetic and thermodynamic consistency appears to be much less understood when diabatic effects and/or a nonlinear equation of state are retained, because the thermodynamics/dynamics coupling then becomes less trivial. In this respect, the oceanographic case is instructive, as oceanographers have used the Boussinesq hydrostatic approximation in conjunction with a realistic nonlinear equation of state (including the pressure dependence) for many decades as the basis for numerical ocean general circulation models of the kind used in climate studies, without any apparent obvious drawbacks apart from the lack of a well-defined and closed energy budget, see Tailleux (2010). Since Boussinesq ocean models appear to work well with a “compressible” equation of state, one may wonder how essential the assumptions of “incompressibility” or “weak compressibility” are in the construction of the Boussinesq and anelastic approximations in the first place.

To clarify this issue, a thermodynamics perspective is useful. Indeed, from a thermodynamic viewpoint, the very idea that it might be possible to simplify a particular equation of state to eliminate its dependence upon pressure while retaining its dependence upon temperature appears to become very dubious if not outright physically meaningless when diabatic effects are retained. This is because the way changes in density are affected by pressure changes depends critically on the particular thermodynamic transformation undergone by the fluid parcels. Take an isothermal transformation for instance.
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(2010) shows that the isothermal compressibility $\gamma = \rho^{-1} \partial \rho/\partial P|_T$ is linked to the adiabatic compressibility $\rho^{-1} \partial \rho/\partial P|_T$ = $1/(\rho c_p^2)$ (his Eq. A.6) by:

$$\gamma = \frac{1}{\rho} \left. \frac{\partial P}{\partial \rho} \right|_{T,S} = \frac{1}{\rho c_p^2} + \frac{\alpha^2 T}{\rho c_p} = \frac{1}{\rho c_p^2} + \alpha \Gamma,$$

(1.1)

where $\Gamma = \alpha T/(\rho c_p)$ is the adiabatic lapse rate. The key point here is that setting up the adiabatic compressibility to zero (by taking the zero Mach number limit $c_s = +\infty$), while it makes the fluid effectively “incompressible” for adiabatic motions, fails in general to do so for nonadiabatic transformations if the thermal expansion coefficient $\alpha$ is allowed to remain nonzero. Note that for seawater, typical values are: $1/(\rho c_p^2) \approx 4.10^{-10} Pa^{-1}$, whereas $\alpha \Gamma = \alpha^2 T/(\rho c_p) \approx 7.5 \times 10^{-13} Pa^{-1}$, using $c_s = 1500 \text{m.s}^{-1}$, $\alpha = 10^{-4} \text{K}^{-1}$, $c_p = 4.10^3 \text{J.K}^{-1}.\text{kg}^{-1}$, and $\rho = 10^3 \text{kg.m}^{-3}$. For these values, the limit $c_s = +\infty$ decreases the isothermal compressibility by about two to three orders of magnitude, so that even if it fails to fully eliminate compressibility effects for nonadiabatic motions, it appears nevertheless capable of reducing them considerably. This being said, if one agrees that the very concept of an “incompressible” fluid becomes physically meaningless when diabatic effects are retained, then one may also agree that it might not be that essential to set up the adiabatic compressibility to zero in the first place. Historically, the latter approach was originally motivated as a natural way to filter out sound waves, but it is now recognised that imposing $c_s = +\infty$ is not necessarily to filter out sound waves, as such a filtering can be more simply achieved by using a hydrostatically adjusted pressure in the equation of state for density, as discussed by de Szoeke & Samelson (2002).

Whether Boussinesq/anelastic models accurately represent the conversions between mechanical energy and internal energy recently came to attention in relation with the question of how strong would the oceanic overturning circulation and meridional heat transport be, and how much diapycnal mixing would then be supported, if it were possible somehow to suppress the mechanical stirring due to the wind and tides, which has been a controversial issue for the past decade, as reviewed in Tailleux (2009), Tailleux (2010), and Hughes & Young (2009). The resulting configuration is often referred to as horizontal convection, see Hughes & Griffiths (2008) for a recent review on the subject. The reason why understanding the nature of the thermodynamics/dynamics coupling is important in that case is because the steady-state mechanical energy balance reduces to:

$$\int_V P \frac{D V}{D t} \, dm = \int_V \rho \varepsilon_K,$$

(1.2)

which shows that in order to estimate the overall viscous dissipation rate, one has to estimate the overall work of expansion/contraction, where $P$ is the pressure, $V$ is the specific volume, $dm = \rho dV$ is the elementary mass element of a fluid parcel, and $\rho \varepsilon_K$ is the viscous dissipation rate. As discussed by Tailleux (2010), the issue of estimating $B$ for a fully compressible fluid is a subtle one. As shown by Paparella & Young (2010) and others, considerable analytical progress can be achieved for a Boussinesq fluid with a linear equation of state, as in that case, Eq. (1.2) becomes:

$$\int_V g z \kappa \nabla^2 \rho \, dV = \int_V \rho_0 \varepsilon_K \, dV = \kappa g_0 \left[ \langle \rho \rangle_{\text{bottom}} - \langle \rho \rangle_{\text{top}} \right],$$

(1.3)

which can be integrated analytically, where $\kappa$ is the molecular diffusivity, $g_0$ the acceleration of gravity and the terms within brackets are the surface area integrated density at the bottom and top of the oceans respectively. Using typical oceanic values, Wang & Huang (2005) estimated the right-hand side to be $O(15 \text{GW})$, which is at least two orders of magnitude smaller than the mechanical power input due to the wind and tides for instance.
The smallness of this number have been widely interpreted as evidence that the surface buoyancy fluxes could not by themselves be responsible for an overturning circulation and associated meridional heat transport of the observed magnitude.

The smallness of the r.h.s. of Eq. (1.3) had been previously interpreted in the context of stratified turbulence (following Winters & al (1995)) as implying that conversions between internal energy and mechanical energy enter the energetics of turbulent stratified mixing only at second order. Tailleux (2009) argued, however, that the apparent smallness of the thermodynamic/coupling in Boussinesq stratified turbulence actually hides two large and opposite conversions between internal energy (IE) and gravitational potential energy (GPE) that almost exactly cancel out, viz., one conversion transferring IE into background GPE, associated with the smoothing out of the vertical reference temperature gradient and a significant overall volume reduction (assuming that $\alpha$ increases with temperature, as is the case for water), the other conversion dissipating available GPE into IE in a way analogous to the viscous dissipation of kinetic energy (KE) into IE, and associated with the increase of the mean thermodynamic equilibrium temperature of the fluid but with only a negligible overall volume expansion. These results suggest therefore that compressibility effects must increase with the degree of stratification and turbulence, which appears to be supported empirically by the kind of laboratory experiment illustrated in Fig. 1 but have yet to be widely accepted, as most subsequent studies so far, e.g., Winters & Young (2009); Hughes & al. (2009); Nycander (2010) continue to favour the classical view that internal energy and thermodynamics/dynamics coupling play only a minor role in the energetics of turbulent stratified mixing.
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At least two important misconceptions about weakly compressible fluids appear to greatly confuse the understanding of the role of compressible effects in stratified turbulent fluids. The first misconception is associated with the widespread (erroneous) belief that a weak thermodynamics/dynamics coupling is an intrinsic feature of all weakly compressible fluids irrespective of the particular thermodynamic transformations undergone by fluid parcels, whereas as far as we can judge, such a weak coupling is an intrinsic feature of adiabatic motions only, with no physical basis for this to be the case for diabatic motions. The second misconception is associated with the widespread confusion about what a “weakly compressible” or “incompressible” fluid is actually supposed to be. Should such a property pertain to a fluid whose density dependence on pressure is eliminated, as seems to have been the original intention, e.g., Lilly (1996), or with the use of the constraints $\nabla \cdot \mathbf{v} = 0$ or $\nabla \cdot (\rho_0 \mathbf{v}) = 0$, as seems to be increasingly assumed following the realization that Boussinesq and anelastic fluids can be used with nonlinear equations of state? Based on the present analysis, the idea of an incompressible fluid seems to be justified only for a fluid with zero adiabatic compressibility in the context of purely adiabatic motions, but physically meaningless otherwise. Physically, the constraints $\nabla \cdot \mathbf{v} = 0$ and $\nabla \cdot (\rho_0 \mathbf{v}) = 0$ do not imply incompressibility or weak compressibility, in contrast to what is often assumed, because they do not preclude diabatic or adiabatic density changes along fluid trajectories. The new view that emerges from the above arguments is that the Boussinesq and anelastic approximations are actually able to support potentially large compressible effects and conversions between internal energy and mechanical energy. If so, this raises many questions that the present paper seeks to clarify. 1) How do the conversions between internal energy and mechanical energy in a Boussinesq/anelastic fluid compare with that of a fully compressible fluid? Does the answer depend on whether diabatic effects and/or a nonlinear equation of state are retained? 2) Do the Boussinesq and anelastic approximations conform with the first and second laws of thermodynamics? What is the form of the thermodynamic potentials supported by such approximations? How different are they from their exact counterparts? 3) Is it an intrinsic problem that many Boussinesq and anelastic models fail to be energetically and thermodynamically consistent, or can such models be modified to correct the problem? In the latter case, can this be done without modifying the formal order of accuracy of the original Boussinesq/anelastic approximations?

The main purpose of this paper is to provide an answer to all above questions, by showing that the Boussinesq and anelastic approximations can be endowed with well defined energetics and thermodynamics that closely mimic that of the fully compressible Navier-Stokes equations. A couple of recent papers have touched upon some of these issues. Thus, Young (2010) showed, using ideas previously developed by Ingersoll (2005), that the seawater Boussinesq equation have a well-defined conserved energy quantity for an arbitrary nonlinear equation of state, although whether this extends to the diabatic case is not clear. Pauluis (2008) addressed a similar issue for the anelastic approximation for a binary fluid such as moist air, also with a highly nonlinear equation of state, and discussed energy and thermodynamic consistency issues. The above studies, however, did not clearly address the nature of the conversions between mechanical energy and internal energy, which is then addressed here in details. Section 2 provides the general theory. Section 3 applies the result to elucidating the thermodynamics of a Boussinesq fluid with a linear equation of state that has been widely used recently in numerical study of turbulent mixing, as well as in the context of horizontal convection. Section 4 discusses the case of the Boussinesq primitive equations currently used in numerical ocean models. Section 5 summarises and discusses some implications of the results.
2. Thermodynamically consistent and inconsistent Boussinesq/anelastic models

2.1. Some specific examples of inconsistent Boussinesq models

To help set up the context and the motivation for the present work, it is useful to provide some specific examples of energetically and thermodynamically inconsistent Boussinesq approximations, which have played and often continue to play a key role in the theoretical and numerical study of many fluid flows of interest in traditional and geophysical fluid dynamics.

2.1.1. Boussinesq fluid with a linear equation of state

The first Boussinesq model of interest is one that is meant to approximate fluids with an equation of state close to linear, retaining all physical processes apart from sound waves from the largest scales down to the molecular diffusive and dissipative scales. Its governing equations are:

\[
\begin{align*}
\frac{D\mathbf{v}}{Dt} + 1 \frac{1}{\rho_0} \nabla \delta P &= -\frac{g_0(\rho - \rho_0)}{\rho_0} \mathbf{k} + \nu \nabla^2 \mathbf{v}, \\
\nabla \cdot \mathbf{v} &= 0, \\
\frac{DT}{Dt} &= \kappa \nabla^2 T, \\
\rho &= \rho_0 [1 - \alpha(T - T_0)],
\end{align*}
\] (2.1)

where \( \mathbf{v} = (u, v, w) \) is the three-dimensional velocity field, \( \delta P = P - P_0 \) is the pressure anomaly defined relative to the reference Boussinesq pressure \( P_0 = -\rho_0 g_0 z \), \( \rho \) is the density, \( T \) is the temperature, \( \rho_0 \) and \( T_0 \) are reference constant density and temperature, \( \mathbf{k} \) is the unit normal vector pointing upwards in the direction opposite to gravity, and \( g_0 \) is a nominal value of the acceleration of gravity. Although such a model is neither energetically nor thermodynamically consistent, as made clear in this paper, it has nevertheless been extensively used in recent theoretical discussion of the energetics of horizontal convection, e.g., [Paparella & Young (2002), Wang & Huang (2005) and Winters & Young (2009)], as well as in discussing the energetics of turbulent mixing in stratified fluids by [Winters & al (1995)]. Moreover, such a model also forms the basis for numerous direct numerical simulations of stratified turbulence, in the sense that in such studies, both \( \kappa \) and \( \nu \) are usually interpreted as representing the molecular values of diffusivity and viscosity respectively. From a thermodynamic viewpoint, the physical meaning of the temperature \( T \) is ambiguous, since it is conserved for adiabatic motions as if it were potential temperature, while also being homogenised by molecular diffusion as if it were in-situ temperature. Regarding pressure, it can be written as the sum of a purely hydrostatic component plus a perturbation \( P' \) that can be regarded as the Lagrange multiplier associated with the incompressibility condition \( \nabla \cdot \mathbf{v} = 0 \), and hence differs from the thermodynamic pressure.

2.1.2. Coarse-grained Boussinesq model with parameterised turbulent fluxes

A second important class of Boussinesq model is that associated with the kind of hydrostatic primitive equations model that has formed the basis for most numerical ocean models currently in used for climate change studies. An early formulation, following that introduced by [Bryan (1969)], is the following:

\[
\begin{align*}
\frac{D\mathbf{u}}{Dt} + f \mathbf{k} \times \mathbf{u} + \frac{1}{\rho_0} \nabla_h \delta P &= A_H \nabla^2_h \mathbf{u} + A_v \frac{\partial^2 \mathbf{u}}{\partial z^2},
\end{align*}
\] (2.5)
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\[ \frac{1}{\rho_0} \frac{\partial \delta P}{\partial z} = -g_0 \left( \frac{\rho - \rho_0}{\rho_0} \right), \]  

(2.6)

\[ \nabla_h \cdot \mathbf{u} + \frac{\partial w}{\partial z} = 0, \]  

(2.7)

\[ \frac{D\theta}{Dt} = K_H \nabla_h^2 \theta + K_v \frac{\partial^2 \theta}{\partial z^2}, \]  

(2.8)

\[ \frac{DS}{Dt} = K_H \nabla_h^2 S + K_v \frac{\partial^2 S}{\partial z^2}, \]  

(2.9)

\[ \rho = \rho(\theta, S, P), \]  

(2.10)

where \( \mathbf{u} = (u, v) \) is the horizontal velocity field, \( w \) is the vertical velocity, \( \nabla_h \) is the horizontal nabla operator, \( A_H \) and \( A_V \) represents horizontal and vertical turbulent eddy viscosities, while \( K_H \) and \( K_V \) represent horizontal and vertical turbulent eddy diffusivities. Here, the full nonlinear equation of state for seawater is used, and is usually formulated in terms of salinity \( S \), potential temperature \( \theta \) and pressure \( P \). Regarding the latter, it is worth pointing out that there is currently much debate about whether the Boussinesq pressure \( P_0 = -\rho_0 g_0 z \) or the full hydrostatic pressure \( P \) should be used in the equation of state, see Shchepetkin & McWilliams (2011) for a discussion of this point. Note that turbulent closure schemes in modern versions of primitive equations models are in general significantly more sophisticated than in the above model, see Griffies (2004) for a detailed discussion of current numerical ocean model formulations. Until very recently, it was generally thought impossible for Boussinesq primitive equations models such as the one above to admit a closed energy budget when using a nonlinear equation of state; as a result, numerical and empirical considerations must have been key in controlling the energetics of current numerical implementations of numerical ocean models and hence their numerical stability.

2.2. Dynamical/thermodynamic coupling in Boussinesq/anelastic models

The first step toward constructing an energetically and thermodynamically consistent Boussinesq/anelastic approximation for an arbitrary nonlinear equation of state is to clarify the nature of the coupling between the dynamics and thermodynamics in a Boussinesq/anelastic fluid. In a real fluid, such a coupling is achieved via the work of expansion/contraction which occurs through the term \( PD\mathbf{v}/Dt \), where \( P \) is the total pressure, and \( \mathbf{v} \) the specific volume. To fix ideas, we examine the issue in the context of the following set of equations, which is based on that previously considered by Ingersoll (2005) and Pauluis (2008):

\[ \frac{D\mathbf{v}}{Dt} + \nabla \cdot \left( \frac{\delta P}{\rho_0} \right) = -\left( \frac{\rho - \rho_0}{\rho_0} \right) g_0 \nabla Z + \frac{1}{\rho_0} \nabla \cdot \mathbf{S}, \]  

(2.11)

\[ \nabla \cdot (\rho_0 \mathbf{v}) = 0, \]  

(2.12)

\[ \frac{D\eta}{Dt} = \dot{\eta} = \frac{\dot{q}}{T} = -\frac{1}{\rho_0} \nabla \cdot (\rho_0 \mathbf{F}_\eta) + \dot{\eta}_{\text{irr}}, \]  

(2.13)

\[ \frac{DS}{Dt} = S = -\frac{1}{\rho_0} \nabla \cdot (\rho_0 \mathbf{F}_S), \]  

(2.14)

\[ \rho = \rho(\theta, S, P_0). \]  

(2.15)

The above system of equations is sufficiently general that it also includes the usual Boussinesq approximation \( \rho_0 = \text{constant} \) as a particular case, as is easily verified. For
that reason, Eqs. (2.11-2.15) will be hereafter referred to as the Boussinesq-Anelastic system, or BA system for short, where \( \eta \) is the specific entropy, \( S \) is salinity, \( g_0 \) is a constant acceleration of gravity, \( Z \) is the geopotential height, so that \( g_0 Z = \Phi \) is the geopotential, and \( S \) is the stress tensor. The terms \( \eta = \dot{q}/T \) and \( \dot{S} \) are used as short-hand to denote the diabatic effects affecting \( \eta \) and \( S \). These are further specified in terms of an entropy flux \( \mathbf{F}_\eta \) and irreversible entropy production term \( \dot{\eta}_{irr} > 0 \) in Eq. (2.13), which is the expression of the second law of thermodynamics, as well as in terms of a salt flux in eq. (2.14), so that salt is assumed to be a conservative quantity. It is important to remark at this stage that the definition of buoyancy \( b = -g_0(\rho - \rho_0)/\rho_0 \) is the one that is the most commonly encountered in the literature. This differs, however, from the form \( b = g_0(v - v_0)/v_0 \) assumed by Pauluis (2008) and Young (2010). As shown in this paper, it turns out that the form used by Pauluis (2008) and Young (2010) is the one that should be used in practice, and the one that is the most energetically and thermodynamically consistent.

Before proceeding, it seems important to point out that although Pauluis (2008)’s derivation of the above BA system initially assumes the reference pressure \( P_0 \) to satisfy the classical hydrostatic balance \( \rho_0^{-1}\partial P_0/\partial z = -g_0\partial Z/\partial z \), this is no longer the case in the final energy conserving form of the equations. Indeed, in absence of fluid motion, setting \( P \) and \( \rho \) to zero in Eq. (2.11) shows that \( P_0 \) and \( \rho_0 \) must actually be solution of:

\[
\frac{\partial}{\partial z} \left( \frac{P_0}{\rho_0} \right) = -g_0 \frac{\partial Z}{\partial z},
\]

which can be immediately integrated as: \( P_0 = P_a - \rho_0 g Z \), where \( P_a \) is the assumed constant and spatially uniform atmospheric pressure at \( Z = 0 \). This form is identical to the Boussinesq reference pressure, except for a non-constant \( \rho_0 \). This in turn implies that:

\[
\rho_0 \frac{D P_0}{D t} \rho_0 = D P_0 \rho_0 + \rho_0 P_0 \frac{D v_0}{D t} = \nabla \cdot (P_0 \mathbf{v}) = -\rho_0 g_0 \frac{D Z}{D t} = \frac{D P_{ib}}{D t},
\]

where \( P_{ib} \) is the reference pressure in hydrostatic equilibrium with \( \rho_0 \), which shows that the relative error in \( P_0 \) as compared to \( P_{ib} \), i.e., \( \delta P_0/P_0 = O(\delta \rho_0/\rho_0) \), and is therefore small by assumption. Therefore, even though the anelastic approximation attempts to relax the incompressibility constraint of the Boussinesq approximation, Pauluis (2008)’s energy conserving form does so at the price of distorting the hydrostatic modes of motions, so that it would be of interest to study the dynamical consequences of the BA system in more details, for instance by following Davies & et al. (2003)’s approach. The issue of whether the distortion of the hydrostatic modes, which is not discussed in Pauluis (2008), could invalidate the approach is beyond the scope of this paper, which is primarily concerned with thermodynamic and energetic consistency issues.

In order to discuss the energetics of the BA system, our starting point is the evolution equation for the kinetic energy, obtained in the usual way by multiplying Eq. (2.11) by \( \rho_0 \mathbf{v} \), which after some manipulation can be written as follows:

\[
\rho_0 \frac{D}{D t} \frac{\mathbf{v}^2}{2} + \nabla \cdot (\delta P \mathbf{v} - \rho_0 \mathbf{F}_{ke}) = \rho_0 b \frac{D Z}{D t} - \rho_0 \varepsilon_K,
\]

where the work against the stress tensor has been written as \( \mathbf{v} \cdot \nabla \mathbf{S} = \nabla \cdot (\mathbf{v} \cdot \mathbf{S}) - \rho_0 \varepsilon_K = \nabla \cdot (\rho_0 \mathbf{F}_{ke}) - \rho_0 \varepsilon_K \) as the difference between the divergence of a flux term minus the viscous dissipation term. For instance, in the special case where \( \rho_0^{-1} \nabla \cdot \mathbf{S} = \nu \nabla^2 \mathbf{v} \), then \( \mathbf{F}_{ke} = \nu \nabla \mathbf{v}^2/2 \) and \( \varepsilon_K = \nu (||\nabla u||^2 + ||\nabla v||^2 + ||\nabla w||^2) \). Over the past decade, a number of studies by Ingersoll (2005), Vallis (2006), Pauluis (2008), Young (2010), Nvecander
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(2010), and McIntyre (2010) all followed a similar approach in seeking to establish the energetic consistency of the above BA system, with the studies differing only in minor details and in the particular set of equations considered. Specifically, all these studies approached the problem by introducing the following function:

$$h^\dagger(S, \eta, Z) = h^\dagger_0(S, \eta) - \int_{Z_0}^{Z} b(S, \eta, Z')dZ'$$  \hspace{1cm} (2.19)

obtained by vertically integrating the buoyancy \( b \) regarded as a function of \( Z \) and of the adiabatically conserved variables, so that:

$$\frac{Dh^\dagger}{Dt} = -b \frac{DZ}{Dt} + C_S \dot{S} + C_\eta \dot{\eta},$$  \hspace{1cm} (2.20)

where

$$C_S = \frac{\partial h^\dagger_0}{\partial S} - \int_{Z_0}^{Z} \frac{\partial h^\dagger_0}{\partial S}dZ', \quad C_\eta = \frac{\partial h^\dagger_0}{\partial \eta} - \int_{Z_0}^{Z} \frac{\partial h^\dagger_0}{\partial \eta}dZ'.$$  \hspace{1cm} (2.21)

Then, summing Eqs. (2.18) and (2.20) yields

$$\rho_0 \frac{D}{Dt} \left( \frac{v^2}{2} + h^\dagger \right) + \nabla \cdot (\delta P v - \rho_0 F_{ke} + \rho_0 F_{h^\dagger}) = \rho_0 (C_S \dot{S} + C_\eta \dot{\eta}) - \rho_0 \varepsilon_K.$$  \hspace{1cm} (2.22)

Because the right-hand side \( \mathcal{R} \) of Eq. (2.22) obviously vanishes for adiabatic and inviscid motions, it may be concluded that the quantity \( \rho_0(v^2/2 + h^\dagger) \) should be regarded as the relevant energy quantity being conserved in absence of diabatic and viscous effects. Note that the energy quantity thus constructed is non-unique, since it involves the arbitrary constant of integration \( h^\dagger_0(S, \eta) \) as discussed by Pauluis (2008). In the context of the Boussinesq approximation, both Young (2010) and Nycander (2010) chose \( Z_0 = h^\dagger_0 = 0 \) and referred to \( h^\dagger \) as the “dynamic enthalpy” and “effective potential energy” respectively.

The above proof is incomplete, however, because establishing the energy consistency of the BA system actually requires: (1) Identifying the quantity playing the role of the total energy; (2) Demonstrating that the total energy thus identified is a conservative quantity for both diabatic and adiabatic motions. By contrast, all what the above arguments manage to establish is that the “adiabatic” energy \( v^2/2 + h^\dagger \) is a conservative quantity for adiabatic motions only. When diabatic effects are retained, this adiabatic quantity is obviously created or destroyed owing to the r.h.s. of Eq. (2.22) becoming non-zero, and hence no longer conservative. In that case, the principle of energy conservation calls for the existence of an additional energy quantity \( h^\ast \) obeying an equation of the type:

$$\rho_0 \frac{Dh^\ast}{Dt} + \nabla \cdot (\rho_0 F_{h^\ast}) = -\mathcal{R},$$  \hspace{1cm} (2.23)

involving some energy flux \( \rho_0 F_{h^\ast} \) to be determined, as upon summation with Eq. (2.22), the following conservation equation is obtained

$$\rho_0 \frac{D}{Dt} \left( \frac{v^2}{2} + h^\dagger + h^\ast \right) + \nabla \cdot (\delta P v - \rho_0 F_{ke} + \rho_0 F_{h^\dagger} + \rho_0 F_{h^\ast}) = 0,$$  \hspace{1cm} (2.24)

which now states that the energy quantity \( v^2 + h^\dagger + h^\ast \) is conservative for both diabatic and adiabatic motions, and hence the natural candidate to play the role of the total energy in the BA system.

Physically, the above approach casts the discussion of energetics in terms of the interactions between the adiabatic energy \( v^2/2 + h^\dagger \) and the diabatic energy \( h^\ast \). While
fully compressible fluid takes the form:

\[ \rho \frac{D}{Dt} \left( \frac{v^2}{2} - b(Z - Z_0) \right) + \nabla \cdot (\delta P v - \rho_0 F_{ke}) = -\rho_0(Z - Z_0) \frac{Db}{Dt} - \rho_0 \varepsilon_K, \quad (2.25) \]

or equivalently, in conservative form:

\[ \frac{\partial (\rho_0 E_m)}{\partial t} + \nabla \cdot \left[ \rho_0 \left( E_m + \frac{\delta P}{\rho_0} \right) v - \rho_0 F_{ke} \right] = -\rho_0(Z - Z_0) \frac{Db}{Dt} - \rho_0 \varepsilon_K. \quad (2.26) \]

For comparison, the corresponding evolution equation for the mechanical energy in a fully compressible fluid takes the form:

\[ \rho \frac{D}{Dt} \left( \frac{v^2}{2} + g_0(Z - Z_0) \right) + \nabla \cdot (P v - \rho F_{ke}) = \rho P \frac{Dv}{Dt} - \rho \varepsilon_K. \quad (2.27) \]

In a compressible fluid, mechanical energy and internal energy are coupled in mainly two ways: (i) via a reversible conversion between internal energy and kinetic energy accomplished by the work of expansion/contraction \( PDv/Dt \); (ii) the irreversible dissipation of kinetic energy into heat by viscous processes \( \varepsilon_K \), as seen in the r.h.s. of Eq. (2.27). Since viscous dissipation is obviously present in both Eqs. (2.25) and (2.27), the only question that needs addressing is whether the following equivalence can be established?

\[ -\rho_0(Z - Z_0) \frac{Db}{Dt} \leftrightarrow \rho P \frac{Dv}{Dt} \quad ? \quad (2.28) \]

To see that this is indeed the case, we expand the pressure and specific volume as follows:

\[ P = P_a - \rho_0 g_0 Z + \cdots, \quad v = \frac{1}{\rho_0} - \frac{\rho - \rho_0}{\rho_0^2} + \cdots \quad (2.29) \]

which uses the underlying assumption in the Boussinesq and anelastic approximations that \((\rho - \rho_0)/\rho_0 \ll 1\). This implies in turn that at leading order, the work of expansion/contraction can be approximated by:

\[ \rho P \frac{Dv}{Dt} \approx \rho_0(P_a - \rho_0 g_0 Z) \frac{D}{Dt} \left( \frac{1}{\rho_0} - \frac{\rho - \rho_0}{\rho_0^2} \right) \]

\[ = -\rho_0(Z - Z_0) \frac{Db}{Dt} + \rho_0(P_a - \rho_0 g_0 Z) \frac{Dv_0}{Dt}. \quad (2.30) \]
Eq. (2.30) shows that the equivalence Eq. (2.28) is exact in the Boussinesq case $\rho_0 = \text{constant}$, but only approximate in the anelastic case because of the term proportional to $D\rho_0/Dt$. This suggests, therefore, that the term $\delta W_{ba} = (Z - Z_0)db$ is the natural counterpart of the compressible work $\delta W = -Pd\nu$ for a compressible fluid. The possibility to identify $\delta W_{ba}$ with $\delta W$ is a key result of this paper, for it points to a natural way to construct the whole range of known thermodynamic potentials for a BA fluid, as shown in the next subsection 2.3. To be fair, the identification of $\delta W_{ba}$ with $\delta W$ is not entirely new, since it was pointed out in earlier studies such as Winters & al (1995), Wang & Huang (2005) and Nycander & al. (2007) for the kind of Boussinesq fluid with a linear equation of state discussed in Section 3. As far as we are aware, however, its consequences for constructing thermodynamically consistent Boussinesq and anelastic approximations do not appear to have been realized until now. Physically, Eq. (2.28) can be interpreted as expressing the fact that in a BA fluid, the compressible work manifests itself through the apparent changes in gravitational potential energy due to the apparent changes in the mass element $dm = \rho dV$, which is possible since a BA fluid conserves the reference mass element $dm_0 = \rho_0 dV$ rather than $dm$.

2.3. Thermodynamics of Boussinesq and Anelastic binary fluids

Having established in the previous section that the energetics of both the Boussinesq and anelastic equations possess a term that can be identified as a conversion between internal energy and mechanical energy, it then becomes relatively straightforward to show that this can be used to construct energetically and thermodynamically consistent BA system of equations. To that end, let us first recall that a basic tenet of classical equilibrium thermodynamics is that the specific internal energy $e = e(\eta, S, \nu)$ of any fluid in local thermodynamic equilibrium (LTE) can be regarded as a function of state whose value is independent of the thermodynamic path followed, where $\eta$ is the specific entropy, $S$ is salinity (the argument would also work if $S$ was the total mixing ratio, as for the case of moist air considered by Pauluis (2008)), and $\nu$ is the specific volume. As is well known, this implies that the reversible work transfer $\delta W = -Pd\nu$ and generalised heat transfer $\delta Q = Td\eta + \mu dS$ entering the total differential of $e$, viz.,

$$de = \delta Q + \delta W = Td\eta + \mu dS - Pd\nu,$$

(2.31)
cannot be specified independently of each other. In classical equilibrium thermodynamics, this interdependence is imposed by the so-called Maxwell relationships, which simply express the result that the cross-derivatives with respect to two different variables must be equal for twice continuously differentiable functions. In the present case, the assumption that $e$ is a function of the thermodynamic state only implies that:

$$T = \frac{\partial e}{\partial \eta}, \quad \mu = \frac{\partial e}{\partial S}, \quad P = -\frac{\partial e}{\partial \nu}, \quad (2.32)$$

which in turn implies the following three Maxwell relationships:

$$\frac{\partial T}{\partial \nu} = \frac{\partial^2 e}{\partial \eta \partial \nu} = \frac{\partial P}{\partial \eta}, \quad \frac{\partial T}{\partial S} = \frac{\partial^2 e}{\partial \eta \partial S} = \frac{\partial \mu}{\partial \eta}, \quad \frac{\partial \mu}{\partial \nu} = \frac{\partial^2 e}{\partial S \partial \nu} = -\frac{\partial P}{\partial S}. \quad (2.33)$$

The above remarks suggest that the simplest way to ensure that the BA system is energetically and thermodynamically consistent is to ensure that the approximation to the generalised heat transfer, denoted here by $\delta Q_{ba} = T_{ba}d\eta_{ba} + \mu_{ba}dS_{ba}$, is similarly linked via relevant Maxwell relationships to the approximation to the work transfer identified previously, viz.,

$$\delta W_{ba} = (Z - Z_0)db, \quad (2.34)$$
where the subscript $ba$ was used to denote the approximation to the generalised ‘heat variables and functions’ $T$, $\eta$, $\mu$ and $S$. If so, this would in turn allows one to regard the following expression:

$$
d e_{ba} = T_{ba} d \eta_{ba} + \mu_{ba} d S_{ba} + (Z - Z_0) db, \quad (2.35)
$$
as the natural counterpart of the fundamental relation of thermodynamics Eq. (2.31), and hence as the total differential of the relevant approximation to the internal energy of the ‘BA fluid’, for which the natural variables are entropy $\eta$, salinity $S$, and buoyancy $b$. In practice, however, it is often more convenient to work with pressure $P$ as a dependent variable rather than specific volume, as well as with temperature $T$ rather than entropy $\eta$, which motivates the introduction of additional thermodynamic potentials constructed from Eq. (2.31) by means of the Legendre transform, e.g., Alberty (2001). The most common thermodynamic potentials that are also the most relevant for the present work are the specific enthalpy $h = e + pv$ and the Gibbs free energy $g = e + pv - T \eta$, whose natural dependent variables are $(\eta, S, P)$ and $(T, S, P)$ respectively. From Eq. (2.35), it is easy to convince oneself that the corresponding approximations to $h$ and $g$ are given by:

$$
h_{ba} = e_{ba} - b(Z - Z_0) \quad \text{and} \quad g_{ba} = e_{ba} - b(Z - Z_0) - T_{ba} \eta_{ba},
$$
with the following total differentials:

$$
d h_{ba} = d [e_{ba} - b(Z - Z_0)] = T_{ba} d \eta_{ba} + \mu_{ba} d S_{ba} - bdZ \quad (2.36)
$$

$$
d g_{ba} = d [e_{ba} - b(Z - Z_0) - T_{ba} \eta_{ba}] = -\eta_{ba} d T_{ba} + \mu_{ba} d S_{ba} - bdZ. \quad (2.37)
$$

Until now, the above considerations have remained rather formal, and while they indicate that it is in principle possible to construct the full range of known thermodynamic potentials for a BA fluid, they have not addressed the issue of how such potentials might be constructed in practice. To simplify notations, we will usually refrain from using the suffix $ba$ for the dependent variables in the following. We should keep in mind, however, that all thermodynamic variables used in the context of the Boussinesq/anelastic approximations are fundamentally different, even if possibly only very slightly in numerical values, from their actual counterparts.

In the previous approaches by Ingersoll (2005), Pauluis (2008), Young (2010) and Nycander (2010), authors have generally assumed the buoyancy $b = b(\eta, S, Z)$ to be given as a function of the dependent variables considered, typically entropy, salinity and geopotential height $Z$. From Eq. (2.36), this can be integrated with respect to $Z$, viz.,

$$
h_{ba}(\eta, S, Z) = h_{ba}(\eta, S, Z_0) - \int_{Z_0}^{Z} b(\eta, S, Z') dZ', \quad (2.38)
$$
for some reference geopotential height $Z_0$, traditionally taken at the ocean surface in the oceanic case, but this only provides an expression for the specific enthalpy up to an indeterminate function of entropy and salinity, which cannot be specified without additional thermodynamic information about the fluid.

The above problem arises because the knowledge of density alone is insufficient to specify all possible thermodynamic quantities; the heat capacity, for instance, cannot be inferred from density. On the other hand, many thermodynamic potentials have the property of encapsulating all known thermodynamic knowledge about a given fluid, as discussed by Callen (1985). In the following, we show how to obtain the relevant approximations to the Boussinesq/anelastic system directly from two such thermodynamic potentials, the Gibbs function and the enthalpy.


2.3.1. Deriving BA thermodynamic potentials from exact thermodynamic potentials

Given the similarity of the approximate and exact differentials for the internal energy, enthalpy, and Gibbs free energy, it is natural to ask whether it is possible to compute the approximate thermodynamic potentials from their exact counterparts, rather than by integrating the total differential of the approximate thermodynamic potentials. That this is indeed the case is shown first for the Gibbs free energy, which is the thermodynamic potential currently chosen to express all the thermodynamic properties for seawater in the latest standard recently adopted by UNESCO, see [IOC, 2010], as advocated earlier by [Feistel, 2003] for instance. To that end, let us introduce the following function:

\[ g_{\text{ba}} = g_{\text{ba}}(T, S, Z) = g(T, S, P_{\text{hb}}(Z)) + g_0(Z - Z_0) = \tilde{g} + g_0(Z - Z_0), \]  

and verify that its total differential agrees with the above differential relationship for the approximate Gibbs function, where \( g = g(T, S, P) \) is the exact Gibbs free energy expressed in terms of its natural variables \( T, S, \) and \( P \). Note that the approximate pressure used in Eq. (2.39) is the pressure \( P_{\text{hb}} \) in hydrostatic balance with \( \rho_0 \), not the anelastic reference pressure \( P_0 = P_a - \rho_0 g_0 Z \). From the result that \( dg = -\eta dT + \mu dS + \nu dP \), it follows that the total differential of \( g_{\text{ba}} \) is given by:

\[ dg_{\text{ba}} = -\tilde{\eta} dT + \tilde{\mu} dS + g_0(1 - \rho_0 \tilde{\nu}) dZ, \]  

where we used \( dP_{\text{hb}} = -\rho_0 g_0 dZ \), and where the tilde quantities are estimated for the reference pressure \( P_{\text{hb}}(Z) \) instead of the actual pressure, so that \( \tilde{\eta} = \eta(T, S, P_{\text{hb}}(Z)), \tilde{\mu} = \mu(T, S, P_{\text{hb}}(Z)) \) and \( \tilde{\nu} = \nu(T, S, P_{\text{hb}}(Z)) \). Eq. (2.40) is obviously consistent with Eq. (2.37) provided that \( \eta_{\text{ba}}, \mu_{\text{ba}} \) and \( b \) be defined by:

\[ \eta_{\text{ba}} = \tilde{\eta}, \quad \mu_{\text{ba}} = \tilde{\mu}, \quad b = -g_0(1 - \rho_0 \tilde{\nu}) = -g_0 \left( \frac{\tilde{\rho} - \rho_0}{\rho_0} \right). \]  

The key result here is that while \( \eta_{\text{ba}} \) and \( \mu_{\text{ba}} \) are found to be identical to their natural tilded expressions, the density \( \rho \) initially used to defined the buoyancy \( b = -g_0(\rho - \rho_0)/\rho_0 \) is on the other hand found to differ from its natural tilded expression \( \tilde{\rho} \), as Eq. (2.41) shows that:

\[ b = -g_0 \left( \frac{\tilde{\rho} - \rho_0}{\rho} \right) = -g_0 \left( \frac{\rho - \rho_0}{\rho_0} \right), \]  

which implies that:

\[ \rho = \rho_0 \left( 1 + \frac{\tilde{\rho} - \rho_0}{\rho} \right) = \rho_0 \left( 2 - \rho_0 \tilde{\nu} \right). \]  

Interestingly, the definition of the buoyancy in Eq. (2.41) is identical to the one recently proposed by [Pauluis, 2008] and [Young, 2010], but differs from the definition usually adopted in most numerical ocean general circulation models as far as we know.

As seen above, the knowledge of \( g_{\text{ba}} \) is sufficient by itself to determine all possible thermodynamic potentials. Thus, the expressions for the specific internal energy and enthalpy are given by:

\[ e_{\text{ba}}(S, T, Z) = g_{\text{ba}} + b(Z - Z_0) + T_{\text{ba}} \eta_{\text{ba}} = \tilde{g} + (g_0 + b)(Z - Z_0) + T\tilde{\eta}, \]  

\[ h_{\text{ba}}(S, T, Z) = e_{\text{ba}} - b(Z - Z_0) = \tilde{g} + g_0(Z - Z_0) + T\eta, \]  

which provide expressions for the specific internal energy and enthalpy in terms of the Gibbs function natural variables \( T, S, \) and \( Z \), rather than in terms of \( e \) and \( h \)’s natural variables. It is easily verified that the total differential for \( e_{\text{ba}} \) and \( h_{\text{ba}} \) are given by:

\[ de_{\text{ba}} = T d\tilde{\eta} + \tilde{\mu} dS + (Z - Z_0) db, \]  

\[ dh_{\text{ba}} = e_{\text{ba}} - b(Z - Z_0) = \tilde{g} + g_0(Z - Z_0) + T\eta, \]
\[ dh_{ba} = T \, d\tilde{\eta} + \tilde{\mu} \, dS - b \, dZ, \quad (2.47) \]

which can be checked to be in agreement with Eqs. (2.35) and (2.36), thus completing the proof.

While the use of the Gibbs function is the most natural approach when the thermodynamic properties are tabulated as functions of \( T, S, \) and \( P, \) as is currently the case for seawater, e.g., IOC (2010), it is sometimes more convenient, depending on the particular situation considered, to work with different dependent variables and hence with a different “master” thermodynamic potential. For a general discussion of the different ways to compile thermodynamic data, the interested reader is referred to Callen (1985).

The specific enthalpy \( h_{ba} = h(\eta, S, P_0 h(Z)) \), owing to the particularly important role it plays for describing and understanding the energetics of stratified fluids, warrants a separate discussion and is therefore discussed next. To that end, let us introduce the function \( h_{ba} \):

\[ h_{ba} = h(\eta, S, P_0 h(Z)) + g_0 (Z - Z_0) = \tilde{h} + g_0 (Z - Z_0), \quad (2.48) \]

and verify that it is the relevant Boussinesq/anelastic approximation to the specific enthalpy. This is done by taking the total differential of \( h_{ba} \), viz.,

\[ dh_{ba} = \tilde{T} \, d\tilde{\eta} + \tilde{\mu} \, dS + g_0 (1 - \rho_0 \tilde{\upsilon}) dZ = \tilde{T} \, d\tilde{\eta} + \tilde{\mu} \, dS - b \, dZ, \quad (2.49) \]

and checking that it agrees with Eq. (2.36). QED. The corresponding expression for the internal energy \( e_{ba} = h_{ba} + b(Z - Z_0) \) can be written as:

\[ e_{ba} = \tilde{h} + (g_0 + b)(Z - Z_0). \quad (2.50) \]

Its total differential is:

\[ de_{ba} = \tilde{T} \, d\tilde{\eta} + \tilde{\mu} \, dS - \rho_0 g_0 \tilde{\upsilon} \, dZ + (b + g_0) dZ + (Z - Z_0) \, db = \tilde{T} \, d\tilde{\eta} + \tilde{\mu} \, dS + (Z - Z_0) \, db, \quad (2.51) \]

which is again consistent with Eq. (2.35).

As a final remark, let us mention that while the above derivations demonstrate that the BA thermodynamic potentials can be constructed from the knowledge of the exact Gibbs function or enthalpy, integration of the Maxwell relationships will in general be needed to construct the BA thermodynamic potentials when an idealised equation of state is assumed. Sections 3 and 4 illustrate in details the two different possible cases.

2.4. Consequence for energy conservation and “heat”-related quantities

The above results make it possible to write down the evolution equations for the specific internal energy and enthalpy by combining Eqs. (2.46) and (2.47) with the evolution equations Eqs. (2.13) and (2.14) for \( \eta \) and \( S \) respectively, leading to:

\[ \rho_0 \frac{D e_{ba}}{Dt} = \rho_0 [\dot{q} + \tilde{\mu} \dot{S}] + \rho_0 (Z - Z_0) \frac{Db}{Dt}, \quad (2.52) \]

\[ \rho_0 \frac{D h_{ba}}{Dt} = \rho_0 [\dot{q} + \tilde{\mu} \dot{S}] - \rho_0 b \frac{DZ}{Dt}. \quad (2.53) \]

Interestingly, taking the difference between these two equations yields the evolution equation for the gravitational potential energy \( b(Z - Z_0) \):

\[ \rho_0 \frac{D}{Dt} [b(Z - Z_0)] = \rho_0 \frac{D(h_{ba} - e_{ba})}{Dt}, \quad (2.54) \]

which shows that for a BA fluid, the gravitational potential energy can be regarded as a thermodynamic property of the fluid, since it is entirely determined from the knowledge of \( S, T, \) and \( Z \). There are therefore two main ways to describe the coupling between dynamics and thermodynamics in a BA fluid, the first one focusing on the coupling
between internal energy and the total mechanical energy (the sum of kinetic energy and gravitational potential energy), and the other between the kinetic energy and the total potential energy (the sum of internal energy and gravitational potential energy, which is equal to the enthalpy here). By combining either one of Eqs. (2.52) or (2.53) with the mechanical energy equation Eq. (2.25), the two following equivalent evolution equations for the total energy

\[ E_t = \frac{v^2}{2} + e_{ba} - b(Z - Z_0) = \frac{v^2}{2} + h_{ba} \]

are obtained:

\[ \rho_0 \frac{D}{Dt} \left[ \frac{v^2}{2} - b(Z - Z_0) + e_{ba} \right] + \nabla \cdot [\delta P \mathbf{v} - \rho_0 \mathbf{F}_{ke}] = \rho_0 \left[ \dot{q} + \dot{\mu} \dot{S} - \varepsilon_K \right], \] (2.55)

\[ \rho_0 \frac{D}{Dt} \left[ \frac{v^2}{2} + h_{ba} \right] + \nabla \cdot [\delta P \mathbf{v} - \rho_0 \mathbf{F}_{ke}] = \rho_0 \left[ \dot{q} + \dot{\mu} \dot{S} - \varepsilon_K \right]. \] (2.56)

Now, in order for the BA system to be energetically consistent, it remains to verify that Eqs. (2.55) and (2.56) are consistent with the principle of energy conservation. This is easily shown to be the case only if the right-hand side of Eq. (2.55) is the divergence of some energy flux \( \mathbf{F}_q \), i.e.,

\[ \rho_0 (\dot{q} + \dot{\mu} \dot{S} - \varepsilon_K) = -\nabla \cdot (\rho_0 \mathbf{F}_q). \] (2.57)

As we show now, this imposes a constraint on the form of the entropy flux \( \mathbf{F}_q \) and irreversible entropy production \( \dot{\eta}_{irr} \) in Eq. (2.13). Assuming salt to be conservative quantity, and hence such that \( \rho_0 \dot{S} = -\nabla \cdot (\rho_0 \mathbf{F}_S) \) for some salt flux \( \mathbf{F}_S \), implies for the evolution equation of specific entropy:

\[ \rho_0 D_{h_{ba}} = \rho_0 \dot{q} = \rho_0 \varepsilon_K + \mu \nabla \cdot (\rho_0 \mathbf{F}_S) - \nabla \cdot (\rho_0 \mathbf{F}_q) \]

\[ = \frac{\rho_0 \varepsilon_K}{T} - \nabla \left[ \frac{\rho_0 (\mathbf{F}_q - \dot{\mu} \mathbf{F}_S)}{T} \right] + \rho_0 \left[ \mathbf{F}_q \cdot \nabla \left( \frac{1}{T} \right) - \mathbf{F}_S \cdot \nabla \left( \frac{\dot{\mu}}{T} \right) \right]. \] (2.58)

The latter expression establishes that the entropy flux \( \mathbf{F}_q \) and irreversible entropy production \( \dot{\eta}_{irr} \) in Eq. (2.13) must be related to the salt flux \( \mathbf{F}_S \) and enthalpy/internal energy flux \( \mathbf{F}_q \) by:

\[ \mathbf{F}_q = \frac{\mathbf{F}_q - \dot{\mu} \mathbf{F}_S}{T}, \] (2.59)

\[ \dot{\eta}_{irr} = \frac{\varepsilon_K}{T} + \mathbf{F}_q \cdot \nabla \left( \frac{1}{T} \right) - \mathbf{F}_S \cdot \nabla \left( \frac{\dot{\mu}}{T} \right). \] (2.60)

In non-equilibrium thermodynamics, this is usually the point at which the second law of thermodynamics is then invoked to further constrain \( \mathbf{F}_q \) and \( \mathbf{F}_S \), in order to guarantee that \( \dot{\eta}_{irr} > 0 \), e.g., see de Groot & Mazur (1962). Going back to the evolution equation for internal energy and enthalpy, note that Eq. (2.57) implies:

\[ \rho_0 D_{e_{ba}} = -\nabla \cdot (\rho_0 \mathbf{F}_q) + \rho_0 \varepsilon_K + \rho_0 (Z - Z_0) \frac{D}{Dt} h_{ba}, \] (2.61)

\[ \rho_0 D_{h_{ba}} = -\nabla \cdot (\rho_0 \mathbf{F}_q) + \rho_0 \varepsilon_K - \rho_0 b \frac{DZ}{Dt}, \] (2.62)

so that \( \mathbf{F}_q \) appears as the diffusive flux of internal energy or enthalpy. Both equations can be regarded as equivalent forms of the first law of thermodynamics.
2.5. Alternative forms of the first law of thermodynamics

We now investigate the consequences of the above results for the determination of various temperature variables. Let us first note that from the differential of the Gibbs function:

$$\frac{dg}{dS} = -\frac{\tilde{\eta}}{\tilde{c}_p} dT + \frac{\tilde{\mu}}{\tilde{c}_p} dS - \tilde{\alpha} g_0 dZ,$$

the Maxwell relationships provide the following partial derivatives for the entropy:

$$\frac{\partial \tilde{\eta}}{\partial S} = -\frac{\partial \tilde{\mu}}{\partial T}, \quad \frac{\partial \tilde{\eta}}{\partial Z} = \rho g_0 \frac{\partial \tilde{\alpha}}{\partial T} = g_0 \tilde{\alpha},$$

by defining $\tilde{\alpha} = \frac{\rho_0}{\tilde{c}_p} \frac{\partial \tilde{\eta}}{\partial T}$ as the relevant definition of the thermal expansion coefficient.

Using the well known result that $\frac{\partial \eta}{\partial T} = c_p \frac{dT}{T}$, this implies that we can write:

$$d\eta = \tilde{c}_p \frac{dT}{T} dT - \tilde{\mu} dS + \tilde{\alpha} g_0 dZ \quad (2.63)$$

As a result, it follows that the temperature equation can be written as:

$$\frac{DT}{Dt} = \frac{T}{\tilde{c}_p} \frac{D\tilde{\eta}}{Dt} + \frac{\tilde{\mu}}{\tilde{c}_p} \frac{DS}{Dt} - \frac{\tilde{\alpha} g_0 T}{\tilde{c}_p} \frac{DZ}{Dt}. \quad (2.64)$$

In absence of salinity, this equation takes the simpler form:

$$\frac{DT}{Dt} = \nabla \cdot \left( \kappa \tilde{c}_p \nabla T \right) \frac{T}{\tilde{c}_p} + \varepsilon K T \quad (2.65)$$

by assuming the diffusive heating to be given by the classical Fourier law $\nabla \cdot (\rho_0 F_q) = -\nabla \cdot (\kappa \rho_0 \tilde{c}_p \nabla T)$. This shows that the evolution equation for in-situ temperature in general possesses: a) a term related to molecular diffusion, that is general not-conservative, i.e., it cannot be expressed as the divergence of a flux because $c_p$ is not constant; b) it usually incorporate the Joule heating due to viscous dissipation; c) it possess a term related to change in pressure, which some authors, e.g. Pons & Le Quéré (2005, 2007), call the “piston effect”, and the resultant Boussinesq equations, the thermodynamic Boussinesq equations.

In practice, the pressure effect can be accounted for by constructing evolution equations for the potential temperature or conservative temperature respectively. In order to show how an equation for $\Theta$ can be constructed, it is useful to construct the potential temperature $\theta$ first. By definition, $\theta$ is the temperature that a parcel with temperature $T$ would have if lifted adiabatically to a reference level $Z = 0$. Potential temperature is thus defined as the implicit solution of the following equation:

$$\eta_{ba}(T, S, Z) = \eta_{ba}(\theta, S, 0). \quad (2.66)$$

Differentiating this expression yields:

$$d\eta_{ba} = \frac{\tilde{c}_p}{T} dT - \frac{\partial \tilde{\mu}}{\partial T} dS + \tilde{\alpha} g_0 dZ = \frac{\tilde{c}_p}{\tilde{\theta}} d\tilde{\theta} - \frac{\partial \tilde{\mu}^*}{\partial S} dS, \quad (2.67)$$

where we defined $\tilde{c}_p = c_p(\theta, S, 0)$ and $\tilde{\mu}^* = \tilde{\mu}(\theta, S, 0)$. In the following, we simplify notations by defining $\tilde{c}_p = c_p(\theta, 0)$. This expression shows that it is possible to rewrite the evolution equation for entropy as follows:

$$\frac{\tilde{c}_p}{\tilde{\theta}} \frac{D\tilde{\theta}}{Dt} = \frac{\partial \tilde{\mu}^*}{\partial S} \frac{DS}{Dt} + \frac{D\eta_{ba}}{Dt}. \quad (2.68)$$

In absence of salinity, we can write:

$$\frac{\tilde{c}_p}{\tilde{\theta}} \frac{D\tilde{\theta}}{Dt} = \frac{\nabla \cdot (\kappa \tilde{c}_p \nabla T)}{T} + \varepsilon K T, \quad (2.69)$$
This can be transformed in the following equation for $\theta$,

$$
\frac{D\theta}{Dt} = \nabla \cdot \left( \frac{\kappa \tilde{c}_p \theta \nabla T}{\tilde{c}_p T} \right) + \dot{\theta}_{irr},
$$

(2.70)

where the nonconservative production/destruction of $\theta$ is given by:

$$
\dot{\theta}_{irr} = -\kappa \tilde{c}_p \nabla T \cdot \nabla \left( \frac{\theta}{\tilde{c}_p T} \right) + \frac{\theta \varepsilon}{\tilde{c}_p T}.
$$

(2.71)

In the literature, $\theta$ is often treated as a conservative variable, which consists in neglecting the nonconservative term $\dot{\theta}_{irr}$. Alternatively, one may remark that the equation for $\theta$ can also be written as:

$$
\tilde{c}_p \frac{D\theta}{Dt} = \frac{D\tilde{h}_\theta}{Dt},
$$

(2.72)

where $\tilde{h}_\theta(\phi) = h_b(\eta, 0)$ is the enthalpy a parcel would have if moved adiabatically from $Z$ to $Z = 0$. For this reason, $\tilde{h}_\theta$ was called “potential enthalpy” by McDougall (2003). This allows one to defined a new temperature variable $\Theta$, also conserved for adiabatic motions, such that: $D\tilde{h}_\theta = c_0^p \Theta$, where $c_0^p$ is an arbitrarily defined specific heat capacity representative of $c_p$ at $Z = 0$. McDougall (2003) discusses a possible choice for $c_0^p$ in the oceanic context. As a result, it is possible to write the above equation as:

$$
\frac{D\Theta}{Dt} = \frac{1}{c_0^p} \frac{D\tilde{h}_\theta}{Dt} = \nabla \cdot \left( \frac{\kappa \tilde{c}_p \theta \nabla T}{c_0^p T} \right) + \dot{\Theta}_{irr},
$$

(2.73)

where this time, the nonconservative production/destruction of $\Theta$ is given by:

$$
\dot{\Theta}_{irr} = -\frac{\kappa \tilde{c}_p}{c_0^p} \nabla T \cdot \nabla \left( \frac{\theta}{T} \right) + \frac{\theta \varepsilon}{T}.
$$

(2.74)

McDougall (2003) provides convincing evidence that the nonconservative term $\dot{\Theta}_{irr}$ is significantly smaller than $\dot{\theta}_{irr}$ for the present-day oceans. The relative smallness of $\dot{\Theta}_{irr}$ over $\dot{\theta}_{irr}$ does not appear to be entirely generic though, and should therefore be checked on a case by case basis, as it may depend on the particular fluid considered and on the degree of turbulence present. It is beyond the scope to simplify the equations further, and to discuss when the evolution equation for $\Theta$ can be approximated by the above simple diffusive model using $\kappa \nabla^2 T$.

3. Thermodynamically and energetically consistent model for a Boussinesq fluid with a linear equation of state

In this section, we return to the case of a Boussinesq fluid with a linear equation of state, originally assumed to be governed by Eqs. (2.1-2.4), with the aim of clarifying its thermodynamics, as well as to improve its formulation to make it thermodynamically and energetically consistent.

3.1. Thermodynamic properties of a Boussinesq fluid with a linear equation of state

We first seek to construct the relevant forms of the specific Gibbs function, enthalpy and internal energy, assuming a linear equation of state $\rho = \rho_0[1 - \alpha(T - T_0)]$ and constant specific heat capacity $c_{p0}$, so that the expression for the buoyancy is:

$$
b = \alpha g_0(T - T_0).
$$

(3.1)
We need to decide on whether to interpret $T$ as the potential or in-situ temperature in the equation of state, as we saw above that any thermodynamically consistent formulation must distinguish between the two kinds of temperature. For completeness, the two cases are considered. We first discuss the case where $T$ is the in-situ temperature, deferring the discussion of an equation of state linear in potential temperature to subsection 3.3. This choice amounts to assume that the isothermal compressibility, rather than the adiabatic compressibility, vanishes. From a thermodynamic viewpoint, this is arguably an awkward assumption, because Eq. (1.1) suggest that this endows the fluid with a negative speed of sound, but since sound waves are filtered out, it is unclear whether this is a serious impediment.

The interpretation of $T$ as the in-situ temperature motivates looking for a description of the thermodynamic properties in terms of the specific Gibbs function $g_{ba}$, since the natural variables of the latter are $T$ and $Z$. As seen previously, the total differential of $g_{ba}$ is

$$dg_{ba} = -\eta_{ba} dT - b dZ,$$

which implies:

$$\frac{\partial g_{ba}}{\partial T} = -\eta_{ba}, \quad \frac{\partial g_{ba}}{\partial Z} = -b.$$  \hspace{1cm} (3.2)

The assumption of constant heat capacity provides the additional differential relation:

$$c_{p0} = -T \frac{\partial^2 g_{ba}}{\partial T^2}.$$  \hspace{1cm} (3.3)

The system of partial differential equations Eqs. (3.2) and (3.3) is sufficient to completely specify $g_{ba}$, whose integration yields

$$g_{ba} = -c_{p0} \left[ T \ln \left( \frac{T}{T_0} \right) - T \right] - \alpha g_0 (Z - Z_0) (T - T_0),$$  \hspace{1cm} (3.4)

up to some arbitrary constant of integration. From Eq. (3.2), the following expression for the specific entropy is obtained:

$$\eta_{ba} = -\frac{\partial g_{ba}}{\partial T} = c_{p0} \ln \left( \frac{T}{T_0} \right) + \alpha g_0 (Z - Z_0).$$  \hspace{1cm} (3.5)

This makes it possible to derive an exact expression for the potential temperature $\theta$, which is the implicit solution of the equation $\eta_{ba}(T, Z) = \eta_{ba}(\theta, 0)$, i.e., $c_{p0} \ln \left( \frac{T}{T_0} \right) + \alpha g_0 (Z - Z_0) = c_{p0} \ln \left( \frac{\theta}{T_0} \right) - \alpha g_0 Z_0$, yielding:

$$\theta = T \exp \left\{ \frac{\alpha g Z}{c_{p0}} \right\}.$$  \hspace{1cm} (3.6)

This makes it clear that in order for a model to be thermodynamically consistent, potential temperature is always different from the in-situ temperature. Now, we previously established that the expressions for internal energy and enthalpy were given by:

$$e_{ba} = g_{ba} + b(Z - Z_0) + T \eta_{ba} \quad \text{and} \quad h_{ba} = e_{ba} - b(Z - Z_0) = g_{ba} + T \eta_{ba},$$

yielding therefore the following expressions:

$$h_{ba} = c_{p0} T + \alpha g_0 T_0 (Z - Z_0),$$  \hspace{1cm} (3.7)

$$e_{ba} = c_{p0} \left[ 1 + \frac{\alpha g_0 (Z - Z_0)}{c_{p0}} \right] T.$$  \hspace{1cm} (3.8)

These relations can be written in terms of other variables by using the expression for $\theta$, as well as $b$. For instance, the enthalpy can be written in terms of the potential temperature and $Z$ as follows:

$$h_{ba} = c_{p0} \theta \exp \left\{ -\frac{\alpha g_0 Z}{c_{p0}} \right\} + \alpha g_0 T_0 (Z - Z_0).$$  \hspace{1cm} (3.9)
Energetics and thermodynamics of the Boussinesq/Anelastic approximations

\[ e_{ba} = c_{p0} \left[ 1 - \frac{\alpha g_0 Z_0}{c_{p0}} + \ln \left\{ \frac{\alpha g_0 \theta}{b + \alpha g_0 T_0} \right\} \right] \left( T_0 + \frac{b}{\alpha g_0} \right) \]  

(3.10)

3.2. Improvement of the model energetic and thermodynamic consistency

Having clarified the nature of the thermodynamics and thermodynamic potentials for a Boussinesq fluid with a linear equation, we now turn to the issue of writing down explicitly how to transform the initial formulation into an energetically and thermodynamically consistent one. The main modification introduced is related to the heat equation. Moreover, there is now a distinction between in-situ temperature and potential temperature.

To summarise, the whole model is therefore given as follows:

\[ \frac{Dv}{Dt} + \frac{1}{\rho_0} \nabla \delta P = b k + \nu \nabla^2 v \]  

(3.11)

\[ b = \alpha g_0 (T - T_0) \]  

(3.12)

\[ \nabla \cdot v = 0 \]  

(3.13)

\[ \frac{D\theta}{Dt} = \frac{\theta}{T} \kappa \nabla^2 T + \frac{\theta \varepsilon_K}{c_{p0} T} \]  

(3.14)

\[ T = \theta \exp \left\{ -\frac{\alpha g_0 Z}{c_{p0}} \right\} \]  

(3.15)

Note that we can rewrite the temperature equation as:

\[ \frac{D\theta}{Dt} = \nabla \cdot \left( \frac{\kappa \theta}{T} \nabla T \right) + \dot{\theta}_{irr} + \frac{\theta \varepsilon_K}{c_{p0} T} \]  

(3.16)

where

\[ \dot{\theta}_{irr} = -\kappa \nabla T \cdot \nabla \left( \frac{\theta}{T} \right) = -\frac{\kappa \alpha g_0}{c_{p0}} \frac{\theta}{T} \frac{\partial T}{\partial z} = -\frac{\kappa \alpha g_0}{c_{p0}} \frac{\partial \theta}{\partial z} + \frac{\kappa \alpha^2 g_0^2}{c_{p0}^2} \]  

(3.17)

Note that it is also possible to write the flux entirely in terms of \( \theta \):

\[ \frac{\kappa \theta}{T} \nabla T = \kappa \nabla \theta - \frac{\kappa \alpha g_0 \theta}{c_{p0}} k \]  

(3.18)

which was computed assuming \( Z(z) = z \). Interestingly, these equations introduce the following length scale: \( L = c_{p0}/(\alpha g_0) \). For typical values, \( c_{p0} = 4.10^4 \text{J.kg}^{-1}.\text{K}^{-1} \), \( \alpha = 10^{-4} \text{K}^{-1} \) and \( g_0 = 10 \text{m.s}^{-1} \), which yields: \( L = 4.10^6 \text{m} \). As \( L \) is huge compared to the typical length scales at which molecular diffusion is important, it follows that the nonconservative term is probably negligible.

3.3. Equation of state linear in potential temperature

This section revisits the above results by assuming that the equation of state is linear in \( \theta \) rather than in \( T \), and hence that the adiabatic compressibility vanishes, as is generally implicitly assumed in traditional low Mach number asymptotics. In this case, the buoyancy becomes:

\[ b = \alpha g_0 (\theta - \theta_0), \]  

(3.19)

with \( \alpha_\theta \) the isentropic thermal expansion, which Tailleux (2010) shows (his Eq. A.11) is related to the classical thermal expansion by \( \alpha_\theta = \alpha T/\theta \) for a constant \( c_{p0} \). The use of \( \theta \) as a dependent variable makes it natural to seek a description of the thermodynamic properties of the fluid from the specific enthalpy, since \( \theta \) is closely related to the specific
entropy by \( d\eta_{ba} = c_{p0}d\theta/\theta \), as seen previously. As a result, the total differential of specific enthalpy can be written as:

\[
dh_{ba} = Td\eta_{ba} - bdZ = \frac{Tc_{p0}}{\theta}d\theta - bdZ, \tag{3.20}
\]

which yields the following system of two partial differential equations:

\[
\frac{\partial h_{ba}}{\partial \theta} = \frac{c_{p0}T}{\theta}, \quad \frac{\partial h_{ba}}{\partial Z} = -b = -\alpha_\theta g_0(\theta - \theta_0). \tag{3.21}
\]

The Maxwell relationship for such a system imposes the following integrability constraint:

\[
\frac{\partial}{\partial Z} \left( \frac{c_{p0}T}{\theta} \right) = -\frac{\partial b}{\partial \theta} = -\alpha_\theta g_0, \tag{3.22}
\]

which can be integrated to yield the following expression between \( T \) and \( \theta \):

\[
\frac{T}{\theta} = 1 - \frac{\alpha_\theta g_0 Z}{c_{p0}}, \tag{3.23}
\]

using the fact that by definition, \( T = \theta \) at \( Z = 0 \). By using Eq. (3.22), it becomes straightforward to integrate the partial differential relations Eqs. (3.21) to eventually obtain

\[
h_{ba} = c_{p0} \left[ 1 - \frac{\alpha_\theta g_0 Z}{c_{p0}} \right] (\theta - \theta_0) = \left( \frac{\theta - \theta_0}{\theta} \right) c_{p0}T, \tag{3.24}
\]

up to an arbitrary constant of integration. The expression for the internal energy is therefore given by:

\[
e_{ba} = h_{ba} + b(Z - Z_0) = [c_{p0} - \alpha_\theta g_0 Z_0](\theta - \theta_0), \tag{3.25}
\]

which implies that in the present model, \( \theta \) is in fact a proxy for the specific internal energy. It is useful to note here that because \( c_{p0} \) is constant, the concepts of potential temperature \( \Theta \) and conservative temperature \( \Theta \) coincide.

The evolution equation for temperature is unchanged, while the expression linking \( T \) and \( \theta \) is now given by Eq. (3.23), so that in summary, the thermodynamics is now described by the system:

\[
\frac{D\theta}{Dt} = \frac{\theta}{T} \kappa \nabla^2 T + \frac{\theta \varepsilon_K}{c_{p0}T}, \tag{3.26}
\]

\[
T = \theta \left[ 1 - \frac{\alpha_\theta g_0 Z}{c_{p0}} \right]. \tag{3.27}
\]

As shown in this paper, the diffusive term can be written as the sum of the divergence of a diffusive flux, plus a nonconservative production/destruction term, which are explicitly given by:

\[
\frac{D\theta}{Dt} = \nabla \cdot \left( \frac{\kappa \theta}{T} \nabla T \right) + \dot{\theta}_{irr} + \frac{\theta \varepsilon_K}{c_{p0}T}, \tag{3.28}
\]

where

\[
\dot{\theta}_{irr} = -\kappa \nabla T \cdot \nabla \left( \frac{\theta}{T} \right) = -\frac{\kappa \alpha_\theta g_0/c_{p0}}{[1 - \alpha_\theta g_0 Z/c_{p0}]^2} \frac{\partial T}{\partial z} = -\frac{\kappa \alpha_\theta g_0}{c_{p0}} \left( \frac{\theta}{T} \right)^2 \frac{\partial T}{\partial z} \tag{3.29}
\]

The nonconservative terms have been shown by McDougall (2003) to be very small compared to the diffusive term, so that can be neglected in practice.
In this section, we return to the Boussinesq primitive equations Eqs. (2.5-2.10) that form the basis for most current numerical ocean general circulation models (save for the form of the turbulent parameterisations), with the aim of showing how to modify them in order to make them energetically and thermodynamically consistent.

4. Improved formulation

It should be clear by now from the above results that two main modifications are needed to make the Boussinesq primitive equations (2.5-2.10) energetically and thermodynamically consistent, which are: 1) modification of the definition of buoyancy, 2) addition of the nonconservative terms in the thermodynamic equation Eq. (2.8). The resulting set of modified equations is as follows:

\[
\frac{D\mathbf{u}}{Dt} + f \mathbf{k} \times \mathbf{u} + \frac{1}{\rho_0} \nabla_h \delta P = A_H \nabla_h^2 \mathbf{u} + A_V \frac{\partial^2 \mathbf{u}}{\partial z^2},
\]

\[
\frac{1}{\rho_0} \frac{\partial \delta P}{\partial z} = -g_0 \left( \frac{\tilde{\rho} - \rho_0}{\tilde{\rho}} \right) \frac{\partial \tilde{Z}}{\partial z} = b \frac{\partial \tilde{Z}}{\partial z},
\]

\[
\nabla_h \cdot \mathbf{u} + \frac{\partial w}{\partial z} = 0,
\]

\[
\frac{D\Theta}{Dt} = K_H \nabla_h^2 \Theta + K_v \frac{\partial^2 \Theta}{\partial z^2} + \dot{\Theta}_{irr},
\]

\[
\frac{DS}{Dt} = K_H \nabla_h^2 S + K_v \frac{\partial^2 S}{\partial z^2},
\]

\[
\tilde{\rho} = \rho(S, \Theta, P_0(Z)),
\]

where \( \Theta \) is now assumed to be the conservative temperature, on the basis of McDougall (2003)'s results suggesting that the nonconservative term \( \dot{\Theta}_{irr} \) is significantly smaller for \( \Theta \) than for the potential temperature \( \theta \), resulting in a smaller error in the overall energy budget when this term is neglected. For completeness, we need to provide an explicit expression for \( \dot{\Theta}_{irr} \). To that end, it is first necessary to understand how to evaluate a number of thermodynamic properties for Boussinesq seawater, which is discussed next.

4.2. Thermodynamics of Boussinesq seawater

In contrast to the idealised Boussinesq model of the previous section, the aim of numerical ocean modelling is to achieve realistic simulations, and therefore to use an equation of state that is as realistic as possible. As mentioned earlier, the thermodynamic properties of seawater are currently encapsulated in a Gibbs function, e.g., Feistel (2003), IOC (2010), with natural variables in-situ temperature, salinity, and pressure. It is therefore natural to seek a determination of Boussinesq thermodynamics from the published Gibbs function. The Boussinesq Gibbs function was shown above to be given by:

\[
g_{ba}(T, S, Z) = g(T, S, P_0(Z)) + g_0(Z - Z_0) = \tilde{g} + g_0(Z - Z_0).
\]

As is well known, the specific entropy \( \eta_{ba} \), the relative chemical potential \( \mu_{ba} \), the buoyancy \( \delta \) (and specific volume), and the specific heat capacity \( c_{p,ba} \) can all be obtained from the first and second partial derivatives of \( g_{ba} \) as follows:

\[
\eta_{ba}(T, S, Z) = \tilde{\eta} = -\frac{\partial \tilde{g}}{\partial T},
\]
\[ R. Tailleux \]

\[ \mu_{ba}(T, S, Z) = \hat{\mu} = \frac{\partial \hat{g}}{\partial S} \]  
\( (4.9) \)

\[ b = -\frac{\partial g_{ba}}{\partial Z} = -\frac{\partial \hat{g}}{\partial Z} - g_0 = g_0(\rho_0 \hat{v} - 1), \]  
\( (4.10) \)

\[ c_{pa} = \hat{c} = -T \frac{\partial^2 \hat{g}}{\partial T^2}, \]  
\( (4.11) \)

where the formula for \( b \) was arrived at by using the result that \( \partial g/\partial P = \nu(S, T, P) \). As previously, tilded quantities refer to quantities estimated for the hydrostatic reference pressure \( P_0(Z) \) rather than the full pressure, so that \( \hat{\nu} = \nu(T, S, P_0(Z)) \) for instance.

In order to arrive at an expression for the conservative temperature, we need the expressions for the specific enthalpy \( h_{ba} \) and potential enthalpy \( h_\theta \), which are respectively given by:

\[ h_{ba}(T, S, Z) = g_{ba}(T, S, Z) + T \hat{\eta} = \hat{g} + g_0(Z - Z_0) + T \hat{\eta}, \]  
\( (4.12) \)

\[ h_\theta(T, S, Z) = h_{ba}(\theta, S, 0) = h_r(\theta, S), \]  
\( (4.13) \)

where the potential temperature \( \theta \) is now the implicit solution of \( \eta_{ba}(T, S, Z) = \eta_{ba}(\theta, S, 0) \).

Using the above expressions for the specific entropy and heat capacity, as well as the Maxwell relationships for the Gibbs function, yields the following expression for the total differential of specific entropy:

\[ dh_{\eta} = dh = \frac{\hat{c}_p dT}{T} - \frac{\partial \hat{\mu}}{\partial T} dS + \frac{\partial b}{\partial T} dZ, \]  
\( (4.14) \)

which in turn yields the following expression for the total differential of specific enthalpy:

\[ dh_{ba} = Tdh = \hat{\mu} dS - b dZ = T \left( \frac{\hat{c}_p dT}{T} - \frac{\partial \hat{\mu}}{\partial T} dS + \frac{\partial b}{\partial T} dZ \right) + \hat{\mu} dS - b dZ \]

\[ = \hat{c}_p dT + \left( \hat{\mu} - T \frac{\partial \hat{\mu}}{\partial T} \right) dS + (g_0 \hat{\alpha} T - b) dZ, \]  
\( (4.15) \)

where \( \partial b/\partial T = \rho_0 g_0 \hat{v} / \partial T = g_0 \hat{\alpha} \), by defining the thermal expansion coefficient by \( \hat{\alpha} = \rho_0 \hat{v} / \partial T \). Similarly, the haline contraction coefficient should be defined by \( \hat{\beta} = -\rho_0 \hat{v} / \partial S \). By evaluating the above expression at \( Z = 0 \), we obtain the following expression for the total differential of potential enthalpy:

\[ dh_\theta = \hat{c}_p dT + \left( \hat{\mu}_r - \theta \frac{\partial \hat{\mu}_r}{\partial \theta} \right) dS = c^0_p d\Theta, \]  
\( (4.16) \)

where \( \hat{c}_p = \hat{c}_p(\theta, S, 0) \) and \( \hat{\mu}_r = \hat{\mu}(\theta, S, 0) \). As discussed by McDougall (2003), the conservative temperature is defined such that \( d\Theta = dh_{\theta}/c^0_p \), for some constant representative value of the specific heat capacity \( c^0_p \). The latter expression allows one to express \( d\theta \) in terms of \( d\Theta \) as follows:

\[ d\theta = \frac{c^0_p}{\hat{c}_p} d\Theta - \frac{1}{\hat{c}_p} \left( \hat{\mu}_r - \theta \frac{\partial \hat{\mu}_r}{\partial \theta} \right) dS. \]  
\( (4.17) \)

Now, by evaluating the differential of entropy Eq. \( (4.14) \) at \( Z = 0 \), as well as by using the implicit definition of potential temperature and Eq. \( (4.17) \), it is possible to write down the differential of entropy equivalently in terms of \( \theta \) or \( \Theta \) as follows:

\[ d\hat{\eta} = \frac{\hat{c}_p^\prime}{\hat{\theta}} d\theta - \frac{\partial \hat{\mu}_r}{\partial \theta} dS = \frac{c^0_p}{\hat{\theta}} d\Theta - \hat{\mu}_r dS, \]  
\( (4.18) \)
which in turn allows one to write the total differential of specific enthalpy in terms of the conservative temperature as follows:

\[ dh_{ba} = T d\tilde{\eta} + \tilde{\mu} dS - b dZ = \frac{T c_p^0}{\theta} d\Theta + \left( \tilde{\mu} - \frac{T \tilde{\mu}_r}{\theta} \right) dS - b dZ. \] (4.19)

This result is used next to provide an explicit expression for the nonconservative production of conservative temperature.

### 4.3. Determination of the nonconservative term \( \dot{\Theta}_{irr} \)

As discussed in Tailleux (2010), the determination of \( \dot{\Theta}_{irr} \) follows from the constraint of total energy conservation. In order to see this, let us first derive the evolution equation for the kinetic energy by multiplying the momentum equations by \( v \). After some manipulation, this can be put in the form:

\[ \rho_0 \frac{D u^2}{Dt} + \nabla \cdot (\delta PV - \rho_0 F_{ke}) = \rho_0 b \frac{D Z}{Dt} - \rho_0 \varepsilon_K, \] (4.20)

where the diffusive flux of kinetic energy and viscous dissipation are given by:

\[ F_{ke} = A_H \nabla_h \frac{u^2}{2} + A_v \frac{\partial u^2}{\partial z} k, \] (4.21)

\[ \varepsilon_K = A_h \left[ \| \nabla_h u \|^2 + \| \nabla_h v \|^2 \right] + A_v \left( \frac{\partial u}{\partial z} \right)^2. \] (4.22)

Now, by inserting the evolution equations for \( \Theta \) and \( S \) into Eq. (4.19), it is possible to rewrite the evolution equation for the specific enthalpy as follows:

\[ \rho_0 \frac{D h_{ba}}{Dt} = \frac{T c_p^0}{\theta} \rho_0 \frac{D \Theta}{Dt} + \rho_0 \left( \tilde{\mu} - \frac{T \tilde{\mu}_r}{\theta} \right) dS - b dZ \]
\[ = \nabla \cdot (\rho_0 F_h) - \rho_0 \dot{h}_{irr} + \frac{T c_p^0}{\theta} \rho_0 \dot{\Theta}_{irr} - \rho_0 b \frac{D Z}{Dt}, \] (4.23)

where the diffusive flux \( F_h \) and the irreversible nonconservative term \( \dot{h}_{irr} \) are given by:

\[ F_h = \frac{T c_p^0}{\theta} \left( K_H \nabla_h \Theta + K_v \frac{\partial \Theta}{\partial z} k \right) + \left( \frac{\tilde{\mu} - \frac{T \tilde{\mu}_r}{\theta}}{\theta} \right) \left[ K_H \nabla_h S + K_v \frac{\partial S}{\partial z} k \right], \] (4.24)

\[ \dot{h}_{irr} = K_H \left[ \nabla_h S \cdot \nabla \tilde{\mu}^{**} + \nabla_h \Theta \cdot \nabla_h \left( \frac{T c_p^0}{\theta} \right) \right] + K_v \left[ \frac{\partial S}{\partial z} \frac{\partial \tilde{\mu}^{**}}{\partial z} + \frac{\partial \Theta}{\partial z} \frac{\partial \left( \frac{T c_p^0}{\theta} \right)}{\partial z} \right], \] (4.25)

where \( \tilde{\mu}^{**} = \tilde{\mu} - T \tilde{\mu}_r/\theta \). Finally, an evolution equation for the total energy is obtained by Eqs. (4.20) and (4.23),

\[ \rho_0 \frac{D}{Dt} \left( \frac{v^2}{2} + h_{ba} \right) + \nabla \cdot (\delta P v + \rho_0 F_h - \rho_0 F_{ke}) = \rho_0 \left( \dot{h}_{irr} + \frac{T c_p^0}{\theta} \dot{\Theta}_{irr} - \rho_0 \varepsilon_K \right), \] (4.26)

which shows that the total energy \( u^2/2 + h_{ba} \) is a conservative quantity only if the right-hand side of the later equation vanishes, which yields:

\[ \dot{\Theta}_{irr} = \frac{\theta}{c_p^0 T} \left[ \varepsilon_K + \dot{h}_{irr} \right]. \] (4.27)

This completes the full specification of the modified Boussinesq primitive equations.
4.4. Errors in the energy budget of current OGCMs

The above results imply that there are at least two main sources of error in the global energy budget of current OGCMs, resulting respectively from their use of the buoyancy $b_{ogcm} = -g_0(\tilde{\rho} - \rho_0)/\rho_0$ instead of $b = \rho_0(\tilde{\rho} - \rho_0)/\tilde{\rho}$, as well as from neglecting the irreversible production term $\dot{\Theta}_{irr}$ in the temperature equation (see Tailleux (2010) for relevant expressions when potential temperature is used). Thus, by replacing the buoyancy $b$ by $b_{ogcm}$ in the kinetic energy equation, as well as by neglecting $\dot{\Theta}_{irr}$ in the enthalpy equation, implies for the evolution equation of total energy in current OGCMs to be of the form:

$$\rho_0 \frac{D}{Dt} \left( \frac{v^2}{2} + h_{ba} \right) + \nabla \cdot (\delta P + \rho_0 F_h - \rho_0 F_{ke}) = \rho_0 \dot{E}_{irr}, \quad (4.28)$$

where the right-hand side $\rho_0 \dot{E}_{irr}$ corresponds to the spurious production/destruction of total energy resulting from the inconsistent treatment of the buoyancy and temperature equation. From the above results, its explicit expression is given by:

$$\rho_0 \dot{E}_{irr} = -\rho_0 \left( h_{irr} + \varepsilon_K \right) + \rho_0 (b_{ogcm} - b) w \approx -\rho_0 \left( h_{irr} + \varepsilon_K \right) - \left( \frac{\tilde{\rho} - \rho_0}{\rho_0} \right)^2 \rho_0 w, \quad (4.29)$$

since we have:

$$b_{ogcm} - b = -g_0 \left( \frac{\tilde{\rho} - \rho_0}{\rho_0} \right) + g_0 \left( \frac{\rho - \rho_0}{\tilde{\rho}} \right) = g_0 \left( 2 - \frac{\rho - \rho_0}{\rho_0} \right) \approx - \left( \frac{\tilde{\rho} - \rho_0}{\rho_0} \right)^2. \quad (4.30)$$

Note here that the final form for the error term $\dot{E}_{irr}$ differs significantly from that discussed in Tailleux (2011), because in the latter study, $\dot{E}_{irr}$ was estimated using the non-approximated thermodynamic potentials, resulting in additional spurious sinks/sources of energy. Interestingly, it is important to note that because the term $(b_{ogcm} - b)$ scales as the square of the small Boussinesq parameter $(\rho - \rho_0)/\rho_0$, it follows that the energetically and thermodynamically consistent Boussinesq formulation has the same order of accuracy as the non-consistent formulation. From that viewpoint, it can be said that of all the possible Boussinesq approximations that can be constructed with the same formal order of accuracy, one can be found that is energetically and thermodynamically consistent.

As discussed in Tailleux (2010), errors in the global energy are likely to be of consequence only if they are associated with spurious forces in the momentum equations. Indeed, Tailleux (2010) estimated that the same error $O(10^{-6} \text{W.m}^{-3})$ in the overall energy budget corresponds only to a spurious heat source/sink in the temperature equation that is $O(7.5K/(\text{million years}))$, which is arguably utterly small, whereas it may correspond to spurious positive or negative acceleration in the momentum equations $O(3 \text{m.s}^{-1}/\text{year})$ in the momentum equations, which is in contrast a significant number. On this basis, it appears important to correct the definition of the buoyancy in current OGCMs, but less vital to retain the nonconservative term $\dot{\Theta}_{irr}$. From a practical computational viewpoint, modifying the definition of buoyancy in current OGCM implementations should be rather straightforward, as it amounts to change the integrand in the particular sub-routine estimating the hydrostatic pressure from the knowledge of density. By contrast, evaluating the nonconservative term $\dot{\Theta}_{irr}$ at each grid point at all time steps would be a major undertaking, since it requires the evaluation of many thermodynamic quantities such as $\tilde{\mu}$, $\tilde{\mu}_v$, $\tilde{c}_p$, $\theta$ and $T$. This would be computationally prohibitive, given that the evaluation of density alone already amounts for a significant fraction of the total CPU time owing to its strongly nonlinear character.
5. Summary and discussion

In this paper, we sought to clarify the nature of the conversions between mechanical energy and internal energy supported by the Boussinesq and anelastic approximations, in the general case of a binary fluid with an arbitrary nonlinear equation of state. A key result was to show that the energetics of such approximations possesses a term that can be identified as playing the role of the classical compressible work of expansion/contraction, which manifests itself as apparent changes in gravitational potential energy due changes in density (and hence of mass if the volume is exactly or approximately conserved, as is the case for such approximations). In contrast with a fully compressible fluid, however, the conversion between mechanical energy and internal energy is between GPE and IE rather than between KE and IE. By regarding this term as the Boussinesq/anelastic approximation to the compressible work $\delta W = -P\Delta V$, it is possible to construct the relevant approximation to the “heat” $\delta Q$ in a consistent way by ensuring satisfaction of Maxwell relationships, which upon integration eventually leads to the construction of consistent expressions for the specific internal energy, as well as of the whole range of known thermodynamic potentials, illustrating Bannon (1996)’s statement that the “thermodynamics is slaved to the dynamics”.

The existence of well-defined thermodynamic potentials from which to derive physically consistent expressions for the first law of thermodynamics appears to be sufficient to endow the Boussinesq and anelastic approximations considered in this paper with fully consistent energetics and thermodynamics, even when diabatic effects and a fully nonlinear equation of state for a binary fluid are retained. In the energetically consistent form of the Boussinesq and anelastic approximations, the sum of kinetic energy and enthalpy is a conservative quantity, and hence the natural total energy for the system. As a consequence, the gravitational potential energy can be regarded as the difference between enthalpy and internal energy, and hence as a purely thermodynamic property of the fluid. These ideas were illustrated by showing how two widely used but energetically inconsistent Boussinesq models could be modified to make them fully energetically and thermodynamically consistent. Interestingly, we find that the modifications required to ensure energetic and thermodynamic consistency do not alter the formal order of accuracy of the approximations. In other words, in the space of all Boussinesq and anelastic approximations of a given order of accuracy, one exists that is fully consistent energetically and thermodynamically. It was also showed how to construct explicitly the full range of thermodynamic potentials for Boussinesq and anelastic models, either by integrating Maxwell relationships in the context of idealised models with idealised equations of state and heat capacities, or by approximating the exact thermodynamic potentials when those are known. A direct application of our results is to suggest that current numerical ocean circulation models possess a potentially significant source of error in their momentum equations owing to their use of an incorrect definition of buoyancy, which could in principle be simply corrected by using the correct definition. Interestingly, the improved definition of buoyancy is one that was recently proposed earlier by Pauluis (2008) and Young (2010), but it does not appear to have been realized until now that such a modification was needed to improve the energetic consistency of current OGCMs.

An important implication of our results is to support the earlier suggestion by Tailleux (2009) that the Boussinesq (and hence anelastic) approximations can support large conversions between mechanical energy and internal energy, and therefore compressibility effects significantly larger than previously assumed. Specifically, the point made in Tailleux (2009) is that in the context of turbulent stratified mixing, the apparent irreversible conversion of available GPE into background GPE should not be interpreted as a mechanical
to mechanical energy conversion, as proposed by Winters & al. (1995), but as an irreversible conversion of AGPE into IE. Note, indeed, that on the one hand, Winters & al. (1995) interpret the following energy conversion term:

$$W_{r,laminar} = \int_V g_0 z \kappa \nabla^2 \rho \, dV = \kappa g_0 \left[ \langle \rho \rangle_{\text{bottom}} - \langle \rho \rangle_{\text{top}} \right], \quad (5.1)$$

as a (laminar) conversion of internal energy into background gravitational potential energy, but on the other hand, interpret the following energy conversion term:

$$W_{r,turbulent} = \int_V g z_r \kappa \nabla^2 \rho \, dV - W_{r,laminar} = - \int_V g \kappa \left\| \nabla \rho_r \right\|^2 \, dV - W_{r,laminar}, \quad (5.2)$$

as the irreversible conversion of AGPE into background GPE$_r$, where $z_r = z_r(x, t)$ is the parcel’s position in Lorenz’s reference state, and hence as a mechanical to mechanical energy conversion, on the grounds that $W_{r,turbulent}$ shows up in the evolution equations for AGPE and GPE$_r$ with opposite signs. Yet, both $W_{r,laminar}$ and $W_{r,turbulent}$ are seen to involve terms of the form $gz \kappa \nabla^2 \rho$, which the present paper argues is the one playing the role of the compressible work of expansion/contraction in the Boussinesq/anelastic approximations. For this reason, Tailleux (2009) argue that $W_{r,turbulent}$ actually refers to two different types of energy conversions in the AGPE and GPE$_r$ evolution equations, for which two different notations should be used. Tailleux (2009) used the notation $D(APE)$ to refer to the dissipation of AGPE into IE.

If one accepts the idea that $D(APE)$ and $W_{r,turbulent}$ actually represent two large conversions between AGPE and IE, and between IE and GPE$_r$ respectively, then the question arises as to how these conversions are actually achieved in reality since there is no direct conversion between IE and GPE in the classical description of the energetics of the fully compressible Navier-Stokes equations? With regard to $W_{r,mixing}$, the theory of the hydrostatic adjustment, e.g., Bannon (1995) can be tentatively invoked to speculate on some of the physical mechanisms and processes involved. Physically, localised heating/cooling anomalies due to molecular diffusion must cause localised pressure anomalies, which will propagate as acoustic waves whose energy can be converted into kinetic energy via the compressible work of expansion/contraction and then ultimately into gravitational potential energy via the buoyancy flux $pgw$. If this is what indeed happens, then it is interesting to note that the Boussinesq/anelastic approximations implicitly assumes that of all the internal energy lost to mechanical energy, all of it goes toward increasing the gravitational potential energy, whereas in reality, it seems plausible that some of it could go toward increasing the turbulent kinetic energy, thereby acting as a positive feedback on turbulent mixing. The latter hypothesis warrants further research, as acoustic waves are known to be capable of generating mean flows via acoustic streaming for instance, e.g., see Lighthill (1978a); Vanneste & Bühler (2011). What are the physical mechanisms involved in the opposite conversion whereby AGPE is ultimately dissipated into IE by molecular diffusion is less clear, because physically AGPE can only be converted reversibly into KE by construction. As a result, the only way to dissipate AGPE into IE by molecular diffusive processes seems to require converting AGPE into KE reversibly, then KE into IE reversibly, presumably in the form of acoustic waves, and finally removing the latter by thermal dissipation. The problem with this hypothesis, however, is that thermal dissipation is generally found to be a significantly less effective way to dissipate acoustic waves in liquids than the bulk viscosity, e.g., Lighthill (1978b) (thermal dissipation is more effective in gases, however). However, as the bulk viscosity dissipates the divergent velocity component, it is absent as a dissipation mechanism in the Boussinesq and anelastic approximations. If the physical mechanisms underlying the AGPE dissipa-
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...tion into IE are indeed related to the dissipation mechanisms of acoustic waves, then it is probably not possible to ascertain that only molecular diffusion is involved in reality.

The overall conclusion is that the diabatic effects due to molecular diffusive processes in turbulent stratified fluids seem to give rise to nontrivial and potentially large conversions between mechanical energy and internal energy even in fluids traditionally regarded as incompressible or nearly incompressible, and that such conversions are actually supported by such models as the Boussinesq and anelastic approximations even if this is still largely unappreciated. The main consequences is that thermodynamics, compressible effects, and the divergent component of the fluid velocity play a potentially more important role than traditionally assumed for understanding the physical processes and mechanisms ultimately involved in the energetics of turbulent mixing in stratified fluids. The present results, which suggest that the Boussinesq and anelastic approximations can support large conversions between mechanical energy, help rationalise why such approximations appears to do so well in simulating turbulent stratified flows. On the other hand, the present results also suggest that real turbulent stratified fluids should exhibit differences with Boussinesq and anelastic fluids, as there must be a limit beyond which neglecting the effects of a divergent velocity may become noticeable for instance. Making progress toward clarifying these issues will probably require further detailed analysis of the energetics of the compressible Navier-Stokes equations along the lines recently developed by Tailleux (2009), and direct numerical simulations of turbulent mixing in fully compressible stratified liquid flows resolving acoustic waves emitted by molecular diffusive heating/cooling and their dissipation mechanisms. Laboratory experiments, of the kind illustrated in Fig. [I] might also help.

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